

=>

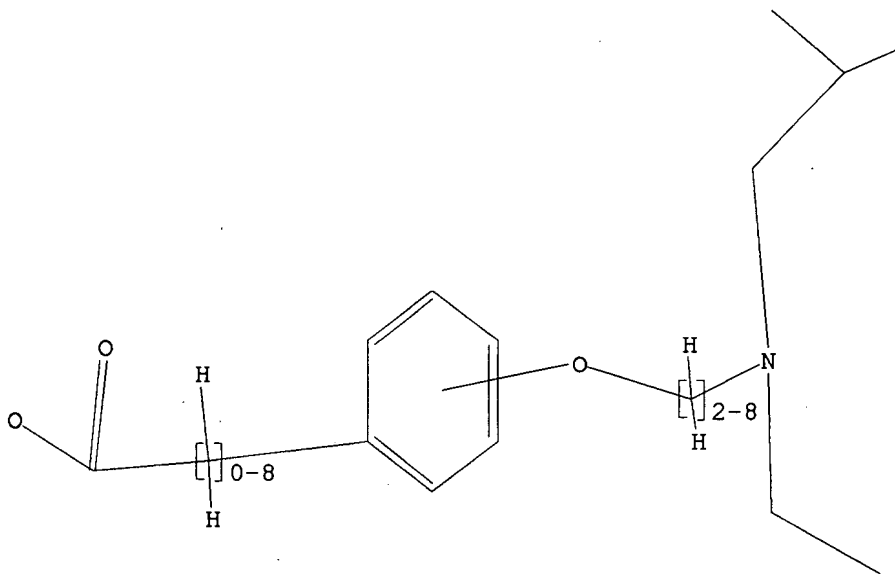
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 12:43:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 40697 TO ITERATE

100.0% PROCESSED 40697 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L2 6 SEA SSS FUL L1

L3 0 L2

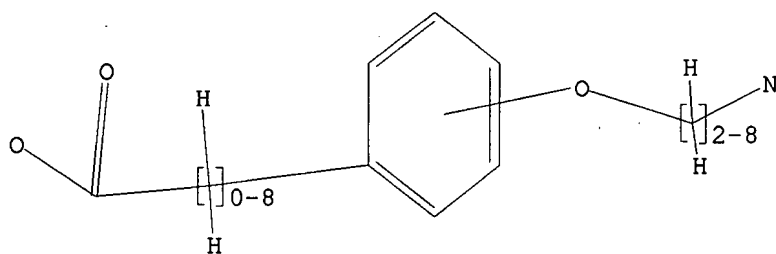
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Uploading C:\Program Files\Stnexp\Queries\8893a.str

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS  
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 12:44:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1888005 TO ITERATE

53.0% PROCESSED 1000000 ITERATIONS

2135 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.16

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 1888005 TO 1888005

PROJECTED ANSWERS: 3840 TO 4220

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L6 375 L5

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21918155 PY<2002

L7 81 L6 AND PY<2002

=> s l7 and phenyl?

849764 PHENYL?

L8 28 L7 AND PHENYL?

=> d 1-28 ibib abs hitstr

L8 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:521702 CAPLUS

DOCUMENT NUMBER: 137:93763

TITLE: Preparation of chiral pyrrolidine derivatives as VLA-4 inhibitors

INVENTOR(S): Nakayama, Atsushi; Machinaga, Nobuo; Yoneda, Yoshiyuki; Sugimoto, Yuichi; Chiba, Jun; Watanabe,

PATENT ASSIGNEE(S): Toshiyuki; Iimura, Shin  
 SOURCE: Daiichi Pharmaceutical Co., Ltd., Japan  
 PCT Int. Appl., 737 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002053534	A1	20020711	WO 2001-JP11641	20011228
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1483024	A	20011228	CN 2001-821484	20011228 <--
CA 2430978	A1	20020711	CA 2001-2430978	20011228
AU 2002219555	A1	20020716	AU 2002-219555	20011228
EP 1346982	A1	20030924	EP 2001-272548	20011228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001016608	A	20040629	BR 2001-16608	20011228
ZA 2003004059	A	20040706	ZA 2003-4059	20011228
CN 1699363	A	20051123	CN 2005-10073706	20011228
RU 2290403	C2	20061227	RU 2003-123115	20011228
IN 2003DN00952	A	20070316	IN 2003-DN952	20030620
MX 2003PA05838	A	20030910	MX 2003-PA5838	20030626
NO 2003002994	A	20030827	NO 2003-2994	20030627
US 2004110945	A1	20040610	US 2003-451159	20030630
US 7157487	B2	20070102		
PRIORITY APPLN. INFO.:			JP 2000-402890	A 20001228
			JP 2001-149923	A 20010518
			CN 2001-821484	A3 20011228
			WO 2001-JP11641	W 20011228
OTHER SOURCE(S):			MARPAT 137:93763	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [WRXM; W = WAA1WB; WA = optionally substituted aryl; A1 = NR1, single bond, C(O); WB = is optionally substituted arylene; R = single bond, NH, OCH2, alkenylene; X = C(O), CH2; M = group represented by the general formula I; R11, R12, R13 each independently = hydrogen, hydroxyl, amino, halogeno; R14 = hydrogen, alkyl; Y = CH2O; Z = optionally substituted arylene; A2 = single bond; R10 = hydroxyl, alkoxy; Q = CH2, S, O, NH], salts thereof, and medicines containing the same are prepared as VLA-4 inhibitors. Title compds. or salts selectively inhibit the binding of cell adhesion mols. to VLA-4 and exhibit high oral absorbability, thus being useful as preventive and/or therapeutic drugs for inflammatory diseases, autoimmune diseases, cancerous metastasis, bronchial asthma, nasal occlusion, diabetes, inflammatory enteric disease, arthritis, etc. The Title compound II was prepared from Et 4-amino-3-chlorophenylacetate, indoline, and Me [(4S)-fluoro-(2S)-pyrrolidinylmethoxy]cyclohexylcarbonate

and the title compound III was prepared from Me 3-hydroxy-4-nitrophenylacetate, Ph isothiocyanate, and Me 4-[(4S)-fluoro-(2S)-pyrrolidinylmethoxy]benzoate.

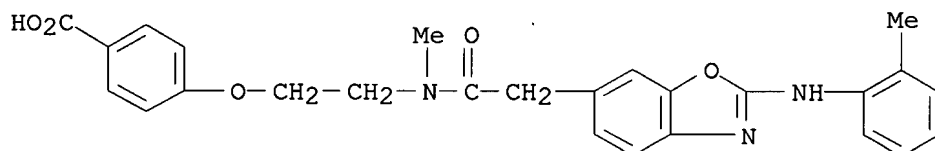
IT 441713-24-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of chiral pyrrolidine derivs. as VLA-4 inhibitors)

RN 441713-24-2 CAPLUS

CN Benzoic acid, 4-[2-[methyl[[2-[(2-methylphenyl)amino]-6-benzoxazolyl]acetyl]amino]ethoxy]- (9CI) (CA INDEX NAME)



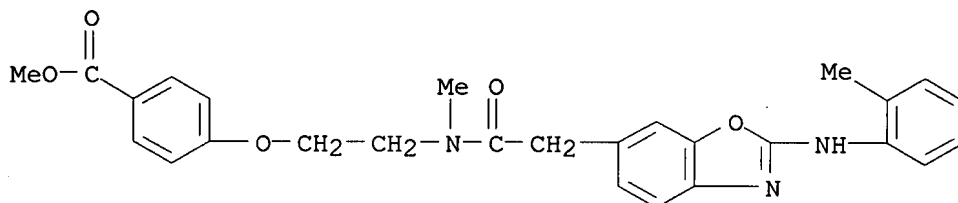
IT 441717-17-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chiral pyrrolidine derivs. as VLA-4 inhibitors)

RN 441717-17-5 CAPLUS

CN Benzoic acid, 4-[2-[methyl[[2-[(2-methylphenyl)amino]-6-benzoxazolyl]acetyl]amino]ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 143 THERE ARE 143 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 28. CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:935587 CAPLUS

DOCUMENT NUMBER: 136:69829

TITLE: Preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents

INVENTOR(S): Kori, Masakuni; Miki, Takashi; Nishimoto, Tomoyuki; Tozawa, Ryuichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd, Japan

SOURCE: PCT Int. Appl., 643 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098282	A1	20011227	WO 2001-JP5347	20010622 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,  
 LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,  
 RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,  
 VN, YU, ZA, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

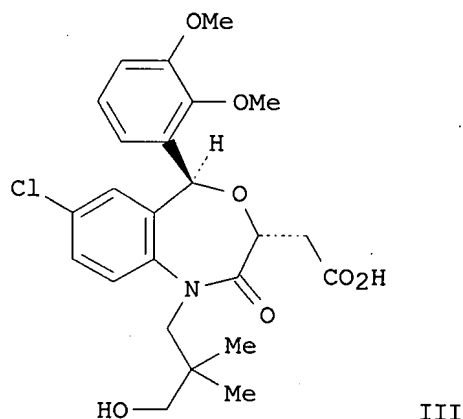
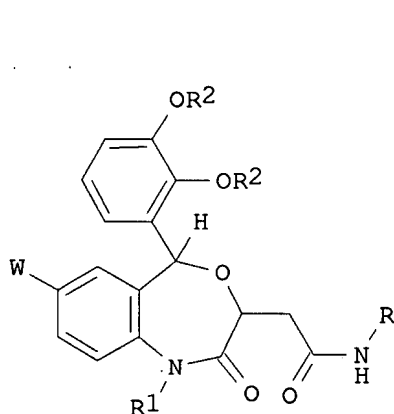
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AU 200174588	A	20020102	AU 2001-74588	20010622
JP 2002080468	A	20020319	JP 2001-189417	20010622
JP 2003064063	A	20030305	JP 2002-233086	20010622
EP 1292585	A1	20030319	EP 2001-941174	20010622

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

BR 2001011835	A	20030429	BR 2001-11835	20010622
HU 2003001301	A2	20030828	HU 2003-1301	20010622
US 2003078251	A1	20030424	US 2002-203524	20020809
ZA 2002009055	A	20031107	ZA 2002-9055	20021107
MX 2002PA12481	A	20030606	MX 2002-PA12481	20021216
NO 2002006164	A	20021220	NO 2002-6164	20021220

PRIORITY APPLN. INFO.: JP 2000-190253 A 20000623  
 JP 2001-189417 A3 20010622  
 WO 2001-JP5347 W 20010622

OTHER SOURCE(S): MARPAT 136:69829  
 GI



AB Alkoxyphenyloxobenzoxazepineacetamides [I; R = (un)substituted 1-carboxyethyl, (un)substituted carboxyalkyl, sulfonylalkyl, (carboxycycloalkyl)alkyl, etc.; R1 = alkyl (un)substituted with alkanoyloxy or OH groups (if R = (un)substituted 1-carboxyethyl, alkyl, 4-carboxycyclohexylmethyl, or 4-carboxyphenylmethyl, then R1 must be substituted with a OH or alkanoyloxy group); R2 = lower alkyl; W = halogen] are prepared as squalene synthase inhibitors for the treatment of hyperlipidemia and the decrease of serum triglycerides and lipids. (3R, 4S)-I [R = Me(CH<sub>2</sub>)<sub>2</sub>SO<sub>2</sub>; R1 = HOCH<sub>2</sub>C(Me)<sub>2</sub>CH<sub>2</sub>; R2 = Me; W = Cl] (II) was prepared in 3 steps from hydroxyacid (III) by acetylation of the hydroxyl group with acetic anhydride, treatment of the acid with thionyl chloride in THF to generate the acid chloride in situ, and addition of the mixture to a solution of PrSO<sub>2</sub>NH<sub>2</sub> in THF to provide the acetylated methoxyphenyloxobenzoxazepineacetamide I [R = PrSO<sub>2</sub>; R1 = AcOCH<sub>2</sub>C(Me)<sub>2</sub>CH<sub>2</sub>; R2 = Me; W = Cl]; hydrolysis of the acetoxy group with aqueous sodium hydroxide and ethanol provides II. Data for the inhibition of squalene

synthase by I are given. Pharmaceutical compns. containing I [R = 3-(HO<sub>2</sub>CCH<sub>2</sub>CH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = HOCH<sub>2</sub>CMe<sub>2</sub>CH<sub>2</sub>; R<sub>2</sub> = Me; W = Cl] are specified.

IT 383667-84-3P 383667-89-8P 383667-94-5P

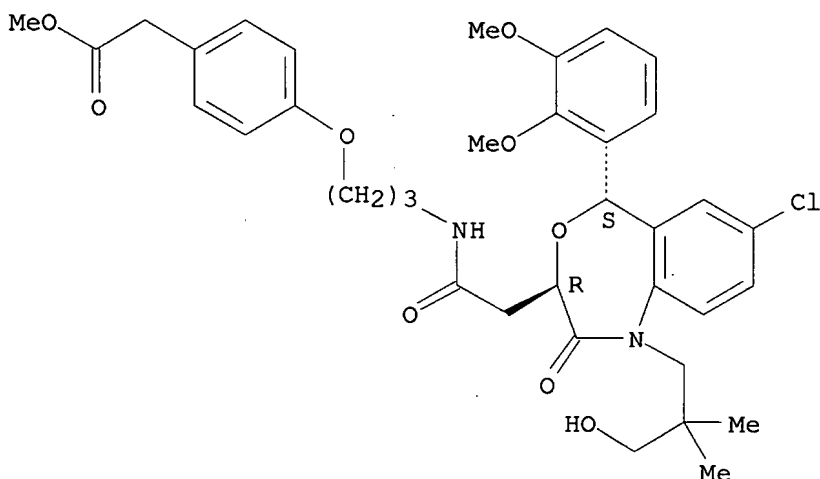
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediates; preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents)

RN 383667-84-3 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, methyl ester (9CI) (CA INDEX NAME)

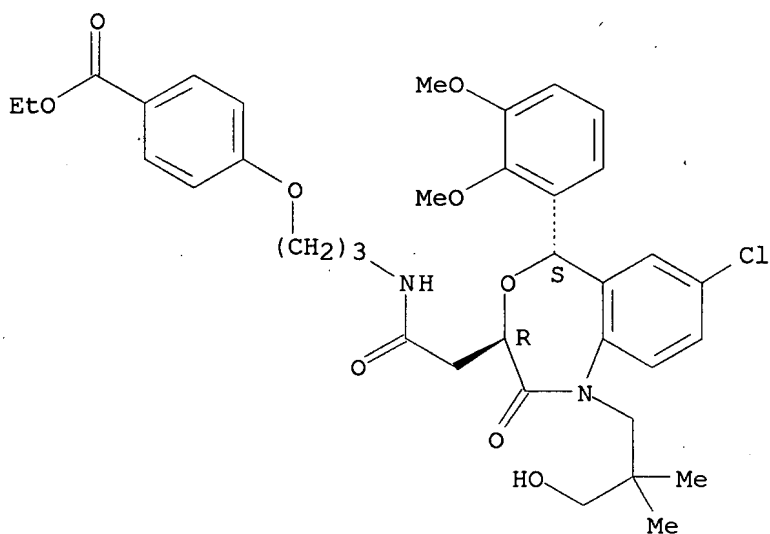
Absolute stereochemistry. Rotation (-).



RN 383667-89-8 CAPLUS

CN Benzoic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, ethyl ester (9CI) (CA INDEX NAME)

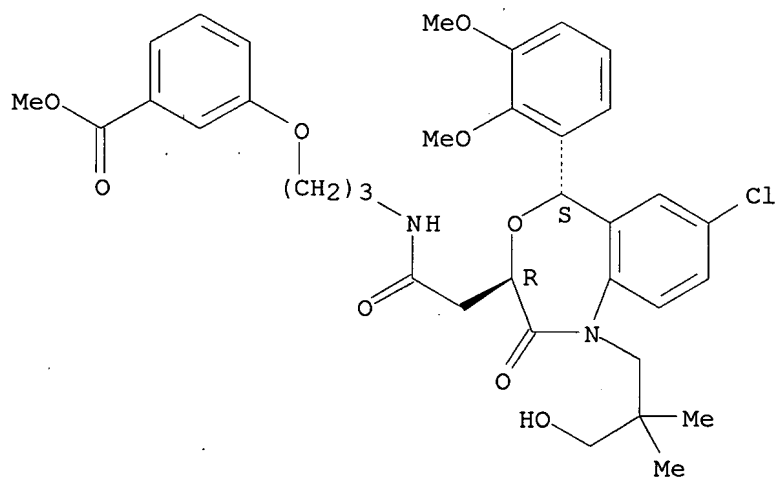
Absolute stereochemistry. Rotation (-).



RN 383667-94-5 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

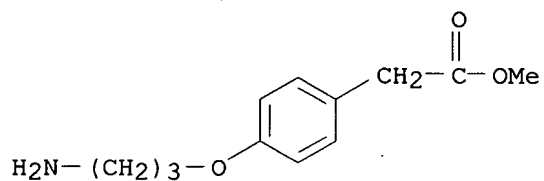


IT 383677-77-8 383677-87-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting materials; preparation of dialkoxyphenyloxobenzoxazepineacetamide  
squalene synthase inhibitors as antihyperlipidemic and  
antihypercholesteremic agents)

RN 383677-77-8 CAPLUS

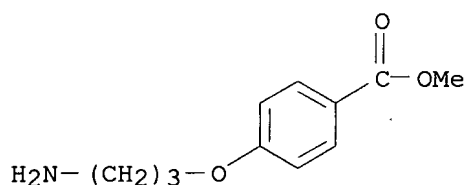
CN Benzeneacetic acid, 4-(3-aminopropoxy)-, methyl ester, hydrochloride (9CI)  
(CA INDEX NAME)



● HCl

RN 383677-87-0 CAPLUS

CN Benzoic acid, 4-(3-aminopropoxy)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

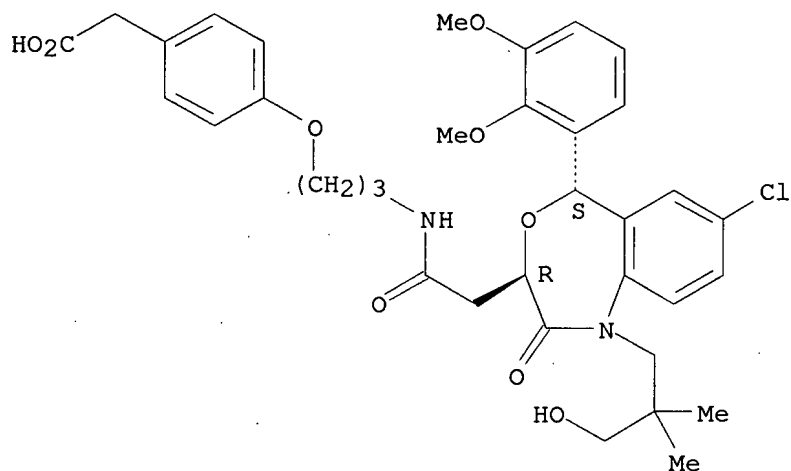
IT 383657-94-1P 383658-05-7P 383658-15-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (title compds.; preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents)

RN 383657-94-1 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

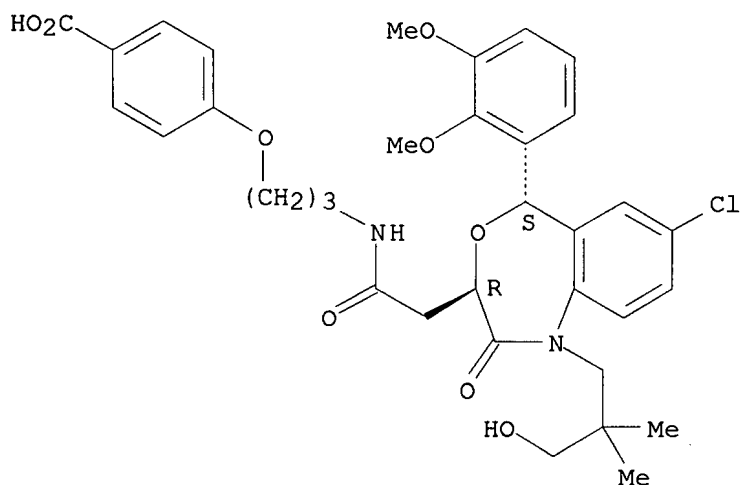
Absolute stereochemistry. Rotation (-).



RN 383658-05-7 CAPLUS

CN Benzoic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

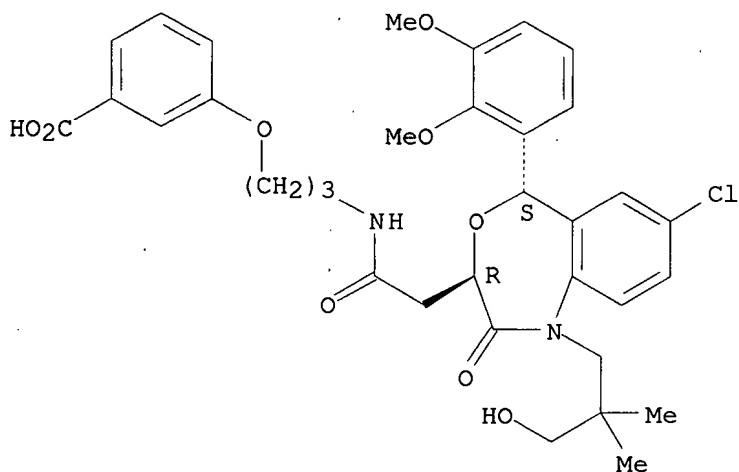
Absolute stereochemistry. Rotation (-).



RN 383658-15-9 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 383657-99-6P 383658-10-4P 383658-20-6P

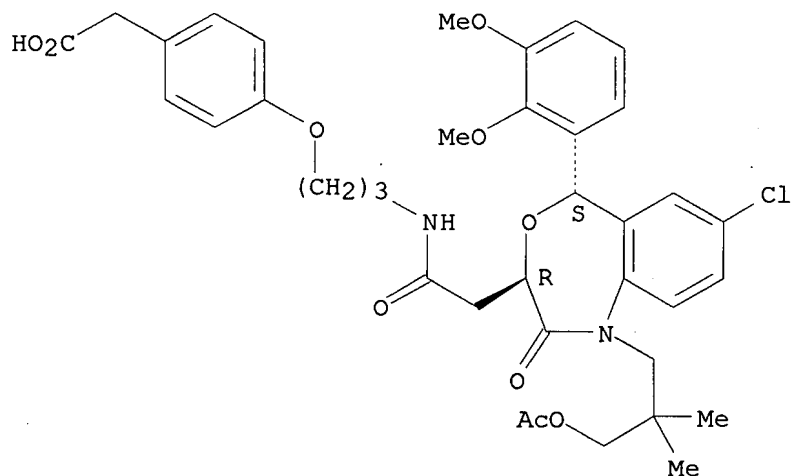
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(title compds.; preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents)

RN 383657-99-6 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

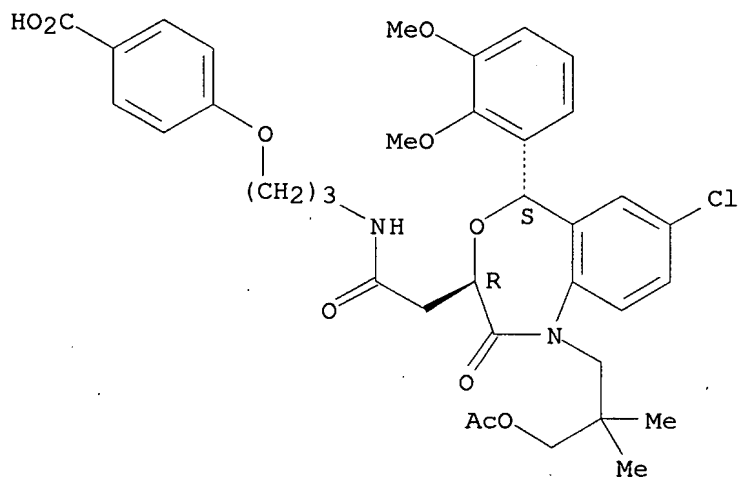
Absolute stereochemistry. Rotation (-).



RN 383658-10-4 CAPLUS

CN Benzoic acid, 4-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

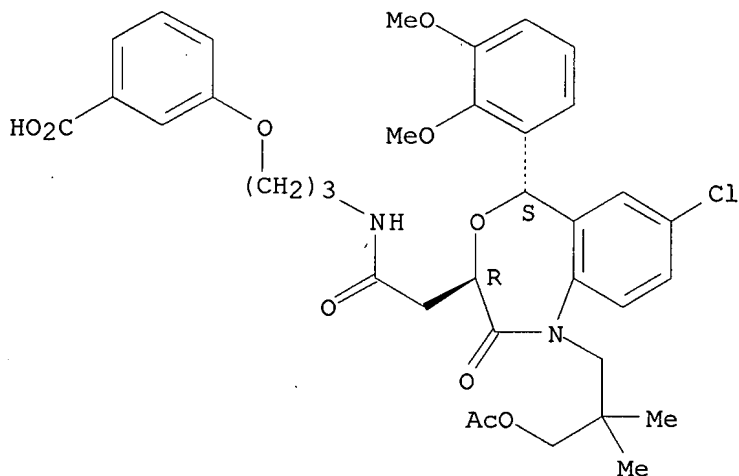
Absolute stereochemistry. Rotation (-).



RN 383658-20-6 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

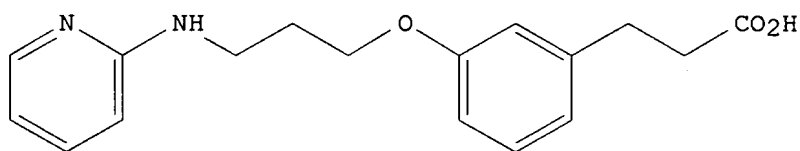
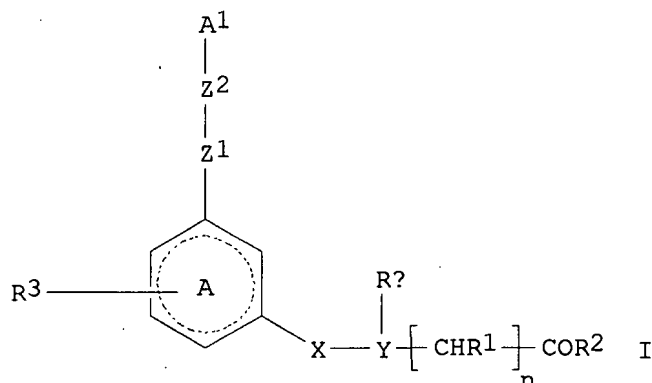
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:923771 CAPLUS  
 DOCUMENT NUMBER: 136:53683  
 TITLE: Preparation of dihydrostilbene alkanolic acid derivatives useful as vitronectin antagonists  
 INVENTOR(S): Rogers, Thomas; Clare, Michael; Fun Lu, Hwang; Russell, Mark; Malecha, James W.; Khanna, Ish Kumar; Penning, Thomas; Nagarajan, Srinivasan Raj  
 PATENT ASSIGNEE(S): Pharmacia Corporation, USA  
 SOURCE: PCT Int. Appl., 163 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001096310	A1	20011220	WO 2001-US19330	20010615 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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AU 2001068490	A5	20011224	AU 2001-68490	20010615 <--
US 2002099209	A1	20020725	US 2001-882137	20010615
US 6720315	B2	20040413		
EP 1289959	A1	20030312	EP 2001-946439	20010615
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JP 2004503540	T	20040205	JP 2002-510453	20010615
US 6833366	B1	20041221	US 2003-657932	20030909
PRIORITY APPLN. INFO.:				
			US 2000-211780P	P 20000615
			US 2001-882137	A3 20010615
			WO 2001-US19330	W 20010615
OTHER SOURCE(S): MARPAT 136:53683				



II

AB The preparation of [I; wherein the "A ring" = 4-8 membered monocyclic, or 7-12 membered bicyclic heteroarene; A1 = 5-9 membered monocyclic, or 7-12 membered polycyclic heterocycle; Z1 = CH<sub>2</sub>, CH<sub>2</sub>O, O, NH, CO, S, etc.; Z2 = 1-5 carbon linker optionally substituted with O, S, or N; X = alkyl, O, amino, CO, etc.; Y = substituted C; R<sub>a</sub> = H, alkyl, alkenyl, etc.; R<sub>1</sub> = H, alkyl, hydroxy, etc.; R<sub>2</sub> = H, alkyl, etc.; R<sub>3</sub> = H, alkyl, halogen, etc.], or a pharmaceutically acceptable salt or composition thereof, and methods of selectively  $\alpha\text{v}\beta 3$  inhibiting or antagonizing the  $\alpha\text{v}\beta 3$  and/or the  $\alpha\text{v}\beta 5$  integrin, are described.

Thus, a multi-step preparation of 3-[[3-(2-pyridinylamino)propoxy]phenyl]propanoic acid II was given. Administration of I inhibits angiogenesis, tumor metastasis, tumor growth, osteoporosis, Paget's disease, humoral hypercalcemia of malignancy, retinopathy, macular degeneration, arthritis, periodontal disease, smooth muscle cell migration, including restenosis and atherosclerosis, and viral diseases.

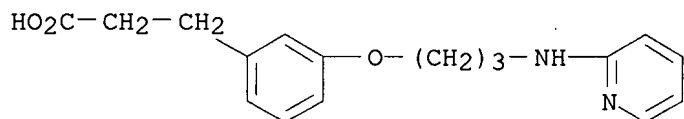
IT 381244-42-4P, 3-[3-[3-(2-Pyridinylamino)propoxy]phenyl]propanoic acid 381244-43-5P, 3-[3-[4-(2-Pyridinylamino)butoxy]phenyl]propanoic acid 381244-44-6P, 3-[3-[5-(2-Pyridinylamino)pentoxyl]phenyl]propanoic acid 381245-59-6P 381245-60-9P 381245-61-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydrostilbene alkanoic acid derivs. useful as vitronectin antagonists)

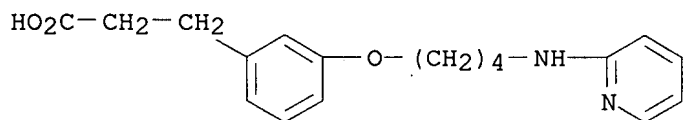
RN 381244-42-4 CAPLUS

CN Benzenepropanoic acid, 3-[3-(2-pyridinylamino)propoxy]- (CA INDEX NAME)



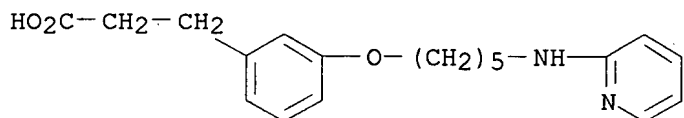
RN 381244-43-5 CAPLUS

CN Benzenepropanoic acid, 3-[4-(2-pyridinylamino)butoxy]- (CA INDEX NAME)



RN 381244-44-6 CAPLUS

CN Benzenepropanoic acid, 3-[[5-(2-pyridinylamino)pentyl]oxy]- (CA INDEX NAME)



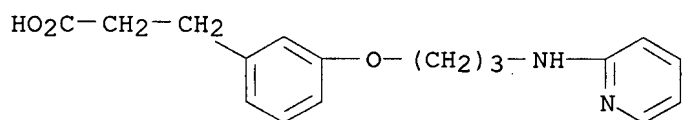
RN 381245-59-6 CAPLUS

CN Benzenepropanoic acid, 3-[3-(2-pyridinylamino)propoxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 381244-42-4

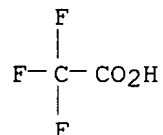
CMF C17 H20 N2 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2

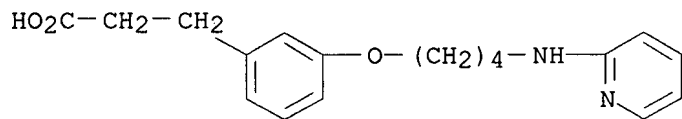


RN 381245-60-9 CAPLUS

CN Benzenepropanoic acid, 3-[4-(2-pyridinylamino)butoxy]-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

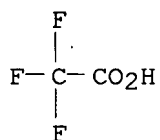
CM 1

CRN 381244-43-5  
CMF C18 H22 N2 O3



CM 2

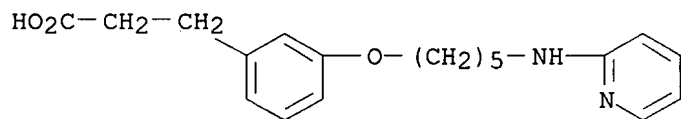
CRN 76-05-1  
CMF C2 H F3 O2



RN 381245-61-0 CAPLUS  
CN Benzenepropanoic acid, 3-[[5-(2-pyridinylamino)pentyl]oxy]-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)

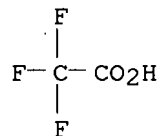
CM 1

CRN 381244-44-6  
CMF C19 H24 N2 O3



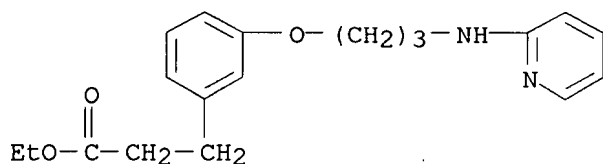
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



IT 381244-81-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of dihydrostilbene alkanonic acid derivs. useful as vitronectin antagonists)  
RN 381244-81-1 CAPLUS  
CN Benzenepropanoic acid, 3-[3-(2-pyridinylamino)propoxy]-, ethyl ester (CA

INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:94262 CAPLUS  
 DOCUMENT NUMBER: 64:94262  
 ORIGINAL REFERENCE NO.: 64:17804g-h,17805a  
 TITLE: Catalyst mixtures for polyurethan reactions  
 INVENTOR(S): Wild, James H.; Williams, Derek  
 PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.  
 SOURCE: 6 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1001458		19650818	GB 1962-45463	19621203 <--

PRIORITY APPLN. INFO.: GB 19621203

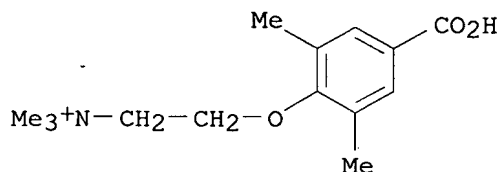
AB The process for treating an organic compound containing two or more reactive NCY radicals in which Y is O or S with a compound containing an active H is accelerated by the use of a mixture of quaternary ammonium, quaternary phosphonium, or ternary sulfonium salt of a strong acid, e.g. Bu3P(Me)I, PhCH2NMe3I, and Me3SI, and an organic metal composition of the type used as catalysts in polyurethan manufacturing These quaternary or ternary salt catalysts are used from 0.05 to 5% by weight of the compound containing active H.

H. The catalysts are salts of acids whose pK value is <4 at 25°. The preferred organic metal polyurethan catalyst compds. are Sn, Zn, or Pb octanoate or Bu2Sn dilaurate.

IT 618880-92-5P, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
 RL: PREP (Preparation)  
 (catalysts, in urethan polymer manufacture)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
 (CA INDEX NAME)



L8 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:20228 CAPLUS  
DOCUMENT NUMBER: 64:20228  
ORIGINAL REFERENCE NO.: 64:3778h,3779a-b  
TITLE: Deactivation of catalyst residues in polyolefins  
INVENTOR(S): Zikmund, Miroslav; Richtrova, Eva; Ambroz, Ludvik  
SOURCE: 4 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 113620		19650215	CS	19630330 <--

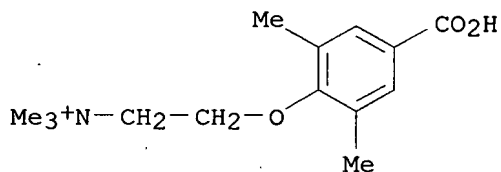
PRIORITY APPLN. INFO.: CS 19630330

AB To a polyolefin heated to 20-100°, a solution of a mixture of alkyl- and arylammonium fluoroantimonates or plumbate (IV) salts of organic acids with an alkyl or arylammonium fluoride and (or) phenyl hydrazinium fluoride, in which alkyl is Me, Et, or Bu, and aryl is Ph or benzyl, in an organic solvent was added (concentration of fluorides 0.1-10 g./kg. of polymer and the weight ratio of plumbates to ammonium or hydrazinium salts was 1:1.2-1.5. Thus, polyethylene was prepared by polymerization in C7H16 with TiCl4 + Et2AlCl at 75°. The suspension of polyethylene was filtered to remove waxlike products and soluble catalyst components. The filtration cake was put in a C7H16 solution containing a 100% molar excess of a complex compound (SbF6)-(NEt4)+ based on Al and Ti in ash. The paste obtained was kept for 3 hrs. at 30° and then the polyethylene was filtered and washed with pure C7H16 and dried. The sheet (0.1 mm.) pressed from the product had good stability.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (in catalyst removal from olefin polymers)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1964:477242 CAPLUS  
DOCUMENT NUMBER: 61:77242  
ORIGINAL REFERENCE NO.: 61:13494c-e  
TITLE: Polymers and copolymers of azo dyes containing vinylsulfone groups  
INVENTOR(S): Grafmueller, Fritz; Weissermel, Klaus  
PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.

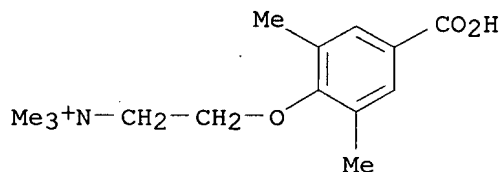
SOURCE: 5 pp.; Addn. to Ger. 1,129,697 (CA 57, 7473b)  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1173652		19640709	DE 1961-F35394	19611121 <--
PRIORITY APPLN. INFO.:			DE	19611121

AB High-mol.-weight polymers were prepared by solution or suspension polymerization

of vinylsulfone group-containing azo dyes of the formula  $H_2C:CHSO_2AN:NRNH_2$ , in which A is an aryl radical which may be substituted in the nucleus by an alkyl or hydroxy alkyl group or a halogen atom, and R is mono- or polysubstituted aryl, pyrazolone, or acetoacetylarylamide radical, in the presence of 0.1-5.0 weight% of an anionic catalyst, based on the weight of the monomer(s), or by the copolymerization of such dyes with other anionic-polymerizable monomers. E.g., benzyltrimethylammonium hydroxide 0.06 in pyridine 2 was added dropwise to 4-aminophenylvinyl sulfone (I) 20 and 4-vinylsulfonyl-2'-methyl-4'-aminoazobenzene (II) 0.5 in pyridine 40 parts. Polymerization set in shortly. During polymerization, the temperature rose from 20 to 50° in spite of cooling, and the mixture became highly viscous. After 3 hrs., the mixture was stirred into MeOH. The copolymer accumulated as a finely divided, bright-red powder. The monomers were removed by extracting the mixture for 24 hrs. (both monomers were MeOH-soluble), and the mixture dried at 70° to yield 20 parts by weight copolymer. The copolymer began to sinter at 170° and changed into a thermoplastic mass at 195-210°, from which filaments could be drawn. It was soluble in HCONMe<sub>2</sub>, Me<sub>2</sub>SO, and α-butyrolactone; the reduced viscosity was 0.08 (in HCONMe<sub>2</sub> at 25°). The color of the polymeric dyes corresponds to that of the monomeric dyes. The reactive basic homo- and copolymers can be used for coloring resins, especially polyesters, polyamides, and polyacetals. They are very heat- and moisture-resistant.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
(catalysts, in polymerization of azo dyes with vinylsulfone groups)  
RN 618880-92-5 CAPLUS  
CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
(CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1964:91269 CAPLUS  
DOCUMENT NUMBER: 60:91269  
ORIGINAL REFERENCE NO.: 60:15986f-h  
TITLE: Asymmetric synthesis of polymers obtained by cationic processes

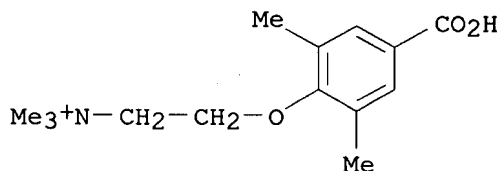
AUTHOR(S): Natta, Giulio; Farina, Mario; Peraldo, Mario; Bressan, Giancarlo  
 CORPORATE SOURCE: Politecnico, Milan  
 SOURCE: Chem. Ind. (Milan) (1961), 43(2), 161-2  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB Benzofuran was polymerized to optically active polybenzofuran (I) by a cationic mechanism. Temps. of -80 to -100° and toluene solvent were used with asym. catalysts, e.g. alkylaluminum halides with optically active acids, alcs., hydroxy acids, amino acids, quaternary ammonium salts, alkaloids, or terpenes. I prepared as above by EtAlCl<sub>2</sub> (II) and (-)-β-phenylalanine, had an intrinsic viscosity (toluene, 30°) = 0.6 dl./g., [α]<sub>D</sub> (2.0% C<sub>6</sub>H<sub>6</sub>) = -33.1, [M]<sub>D</sub> = -39.1 (referred to the monomeric unit), and [M]<sub>303</sub> (dioxane) = -800. I prepared by II and (-)-brucine had [α]<sub>D</sub> = +2.8. I prepared by II and (+)-camphorsulfonic acid had [α]<sub>D</sub> = -3.6. Infrared examination gave a structure for I in which all the C atoms of the chain are asym. I was amorphous on x-ray examination, but is believed to have a head-to-tail and diisotactic structure. The difficulty of crystallization of I is tentatively attributed to steric hindrance. The absence of optically active end groups derived from the catalyst was shown by infrared measurements and the use of 35S-labeled cocatalysts. Optical activity is considered to be induced in I by an asym. counterion.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
 (catalysts from Al compds. and optically-active, in asymmetric polymerization of benzofuran)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
 (CA INDEX NAME)



● Cl<sup>-</sup>

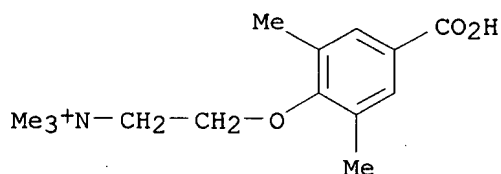
L8 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1964:61387 CAPLUS  
 DOCUMENT NUMBER: 60:61387  
 ORIGINAL REFERENCE NO.: 60:10819a-c  
 TITLE: Catalysts for polymerization of ethylene and propylene  
 PATENT ASSIGNEE(S): Solvay & Cie  
 SOURCE: 7 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 624645		19630509	BE	<--
GB 960086			GB	
PRIORITY APPLN. INFO.:			NL	19611115

AB Relatively low mol. wts. of 30,000-40,000 are achieved by addition of amines

or quaternary ammonium salts to the ternary catalyst (Ziegler type) which consists of: (a) a metal, metal hydride, or an organometallic composition of metals of Groups IV, V, or VI; (b) a compound of a multivalent metal with at least 3 valences; and (c) a halide of an element of Group III or V. For example, (a) may be Bu<sub>4</sub>Sn, (b) TiCl<sub>4</sub>, and (c) AlCl<sub>3</sub>. The amines include Pr<sub>2</sub>NH, PhNH<sub>2</sub>, pyridine, N,N'-diphenyl-p-phenylenediamine, naphthylamine, hexylamine, diphenylguanidine, and sym- or N,N-diethyl-p-phenylenediamine. The quaternary ammonium salts used should be dimethylbenzylammonium, trimethylbenzylammonium, dodecyltrimethylammonium, or octadecyltrimethylammonium chloride, or tetrabutylammonium iodide. Amts. of the addns. vary between 0.01 and 1 mole per g.-atom of the multivalent metal with 3 valencies. For example, C<sub>2</sub>H<sub>4</sub> is polymerized for comparison either with the TiCl<sub>4</sub>Bu<sub>4</sub>Sn-AlCl<sub>3</sub> ternary catalyst or with addns. of 1 of the above amines. Thus, a catalyst is prepared by warming at 25° for 48 min. TiCl<sub>4</sub> 184, Bu<sub>4</sub>Sn 708, and AlCl<sub>3</sub> 245 mg. A suspension of the catalyst is diluted with 1 l. of dry, pure C<sub>6</sub>H<sub>14</sub>. The solution is poured into an autoclave heated to 80° and C<sub>2</sub>H<sub>4</sub> is introduced at 10 atmospheric at a flow rate of 120 g./hr. The polymerization is stopped after 2 hrs. The polyethylenes are washed, dried, and examined. The mol. weight is ascertained by a viscosimetric method. Polymerization without the amine addition gives a polyethylene of mol. weight 55,000; with addition of 20.0 mg. hexylamine/l. C<sub>6</sub>H<sub>14</sub>, the mol. weight is only 37,000.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylol)oxy]ethyl]trimethyl, chloride  
(catalysts, in polymerization of C<sub>2</sub>H<sub>4</sub> and propene, for mol. weight control)  
RN 618880-92-5 CAPLUS  
CN Ammonium, [2-[(4-carboxy-2,6-xylol)oxy]ethyl]trimethyl, chloride (7CI)  
(CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1963:408695 CAPLUS  
DOCUMENT NUMBER: 59:8695  
ORIGINAL REFERENCE NO.: 59:1531d-h,1532a-d  
TITLE: Quaternary ammonium salts from tertiary 2-phenoxyethylamines  
INVENTOR(S): Copp, Frederick C.; Elphick, Albert R.; Coker, Geoffrey G.  
PATENT ASSIGNEE(S): Wellcome Foundation Ltd.  
SOURCE: 13 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 919126		19630220	GB	19580701 <--

GI For diagram(s), see printed CA Issue.

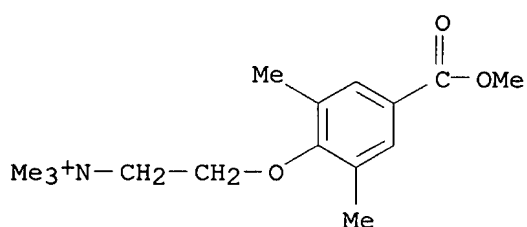
AB (Phenoxyalkyl)dialkylamines are treated with alkyl halides to give I and II, where R and R1 are Me or Et, R2 and R3 are H, halogen, MeO, or Me, Y is NO2, Cl, an alkyl, or an alkoxy group, Z is a Cl-3 alkoxy group, and X is iodine or Br; I and II can be used as depressants for the peripheral sympathetic nervous system. Thus, 136 g. 4-hydroxy-3,5-dimethylbenzophenone is added to a solution of 13.8 g. Na in 950 mL. hot EtOH, 136 g. BrCH2CH2Br added, the mixture refluxed 7 h., approx. 700 mL. EtOH evaporated in vacuo, the residue poured into 500 mL. H2O, the oil that sep. extracted with Et2O, the extract washed with 5N NaOH, the Et2O evaporated, and

the residue distilled to give 2-(4-benzoyl-2,6-dimethylphenoxy)ethyl bromide (III), b0.01 182-6°, m.p. 76°. A mixture of 16.7 g. III and 50 g. 25% Me2NH(MeOH) is heated in a sealed tube at 100° 6 h., the mixture evaporated, excess 5N NaOH added to the residue, the oil that sep. extracted

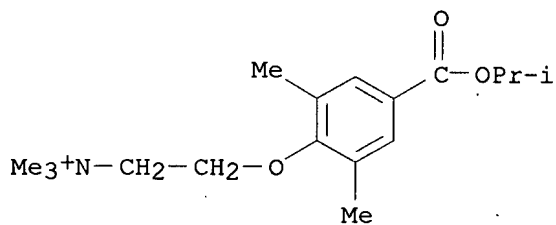
with Et2O, the Et2O evaporated, and the residue distilled to give 1-(4-benzoyl-2,6-dimethylphenoxy)-2-dimethylaminoethane (IV), b0.001 162-7°. MeI (4 g.) is added to a solution of 4 g. IV in Me2CO, the mixture kept 1 h., refluxed 30 min., and cooled to give N-[2-(4-benzoyl-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, m. 208-9° (EtOH). Similarly prepared are I (Y, R2, R3, R, R1, X, m.p. given): H, Me, Me, Me, Et, iodine, 185-6° (EtOH); H, Me, Me, Me, Me, Br, 204-5° (iso-PrOH); p-Me, Me, Me, Me, Me, Br (hemihydrate), 216-17° (EtOH-iso-PrOH); m-Me, Me, Me, Me, Me, Br, 221°; o-Cl, Me, Me, Me, Me, Br, 204-5°; m-Cl, Me, Me, Me, Me, Br, 203-4°; p-Cl, Me, Me, Me, Me, Br, 226-7°; o-MeO, Me, Me, Me, Me, Br, 216-17°; m-MeO, Me, Me, Me, Me, Br, 176-8°; p-MeO, Me, Me, Me, Me, Br, 189-90°; p-EtO, Me, Me, Me, Me, Br, 203°; p-NO2: Me, Me, Me, Me, Br, 240-1°; H, Cl, Cl, Me, Me, Br, 186°, H, H, H, Me, Me, Br, 196-7°; p-NH2, Me, Me, Me, Me, iodine, 239-41°; H, H, Br, Me, Me, iodine, 209-10° (MeOH); H, H, Br, Me, Et, iodine, 165-6°; H, H, Cl, Me, Me, Br, 199-200° (iso-PrOH-Et2O); H, H, F, Me, Me, iodine, 227-80°; H, H, F, Me, Et, iodine (hemihydrate), 211-12°; H, Br, Me, Me, Me, iodine, 178-9° (EtOH-iso-PrOH); H, Me, Et, Me, Et, iodine, 221-2°; H, Me, Me, Me, HO(CH2)2, iodine, 160-1° (EtOH); H, Me, Me, HO(CH2)2, HO(CH2)2, iodine, 110-11°; H, Me, Me, Et, Et, iodine, 149-50° (EtOH); H, H, MeO, Me, Me, iodine, 189-90° (EtOH-ether); H, Me, Me, Me, Me, Cl (hydrate), 209° (iso-PrOH-Et2O); and H, Me, Me, Me, Me, MeSO4, 138-9° (EtOH-EtOAc). Similarly prepared are II (Z, R2, R3, R, R1, X, m.p. given): Me, Me, Me, Me, Me, iodine, 182-3° (EtOH); Et, Me, Me, Me, Me, iodine, 181-2° (EtOH); Et, Me, Me, Me, Et, Br, 109-11° (iso-PrOH-Et2O); PhCH2, Me, Me, Me, Me, Br, 148-50° (iso-PrOH); EtO, H, H, Me, Me, iodine, 157-60° (EtOAc-EtOH); MeO, H, H, Me, Me, iodine, 205-7° (Me2CO-EtOAc); MeO, Me, H, Me, Me, iodine, 149-51° (EtOH-EtOAc); MeO, Me, Me, Me, Me, iodine, 213-15° (EtOH-EtOAc); EtO, H, H, Et, Et, iodine, 128° (EtOH-EtOAc); EtO, Me, H, Me, Me, iodine, 163-5° (EtOH-EtOAc); iso-PrO, Me, Me, Me, Me, iodine, 186-7° (iso-PrOH); MeO, MeO, H, Me, Me, iodine 181-4° (EtOH); EtO, MeO, H, Me, Me, iodine, 136-8° (EtOH); EtO, MeO, MeO, Me, Me, iodine, 208-10° (EtOH); MeO, Br, H, Me, Me, iodine, 196-9° (EtOH); MeO, Br, H, Me, Et, iodine, 186-9° (EtOH); EtO, Br, H, Me, Me, iodine, 184-5° (iso-PrOH); EtO, Br, H, Me, Et, iodine, 121-4° (iso-PrOH); and EtO, Me, Me, Me, Me, iodine, 177-9° (EtOH-EtOAc). Also prepared are (m.p. given) N-[3-(4-benzoyl-2,6-dimethylphenoxy)propyl]-N,N,N-trimethylammonium bromide, 160-1°; N-[2-(4-benzoyl-2,6-dimethylphenoxy)-1-methylethyl]-N,N,N-trimethylammonium iodide, 215-16° (EtOH); N-[2-(4-benzoyl-2,6-dimethylphenoxy)-2-methylethyl]-N,N,N-

trimethylammonium iodide, 167° (EtOH); N-[2-(4-benzoyl-3-hydroxyphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 139-40° (EtOH); N-[2-(4-acetamido-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 242-4° (MeOH); and N-[2-(4-propionylamino-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 197-9° (EtOH).

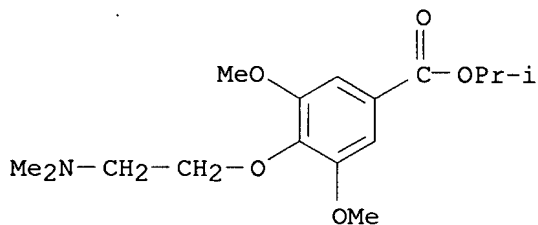
- IT 701193-78-4P, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, Me ester 805949-72-8P, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, iso-Pr ester 875831-55-3P, Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, isopropyl ester  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 701193-78-4 CAPLUS  
 CN Ethanaminium, 2-[4-(methoxycarbonyl)-2,6-dimethylphenoxy]-N,N,N-trimethyl-  
 (CA INDEX NAME)



- RN 805949-72-8 CAPLUS  
 CN Ethanaminium, 2-[2,6-dimethyl-4-[(1-methylethoxy)carbonyl]phenoxy]-N,N,N-trimethyl- (CA INDEX NAME)



- RN 875831-55-3 CAPLUS  
 CN Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, isopropyl ester (7CI) (CA INDEX NAME)



ORIGINAL REFERENCE NO.: 58:14148f  
 TITLE: Cyanoethyl polyamides  
 PATENT ASSIGNEE(S): Romania, Ministry of Petroleum and Chemical Industry  
 SOURCE: 2 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

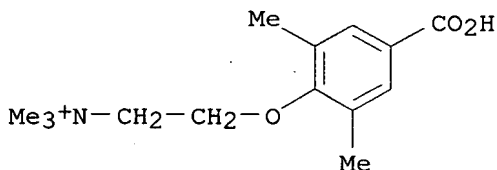
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 920213		19630306	GB 1959-23855	19590710 <--
PRIORITY APPLN. INFO.:			RO	19580712

AB Polyamides are modified by treatment at 20-90° with acrylonitrile (I) in the presence of basic catalysts. Thus, a suspension of 0.4 g. powdered NaOH and 4 g. powdered polycaprolactam (II) in a solution of 10 g. I (stabilized with 0.5% phenyl-β-naphthylamine) in 50 cc. dioxane was heated at 75-7° for 1 hr. Working up resulted in 8.5 g. yellowish powder containing 6.5% nitrile N, 16.3% total N, and 70% cyanoethyl-substituted polyamide units.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (catalysts, in cyanoethylation of polyamides)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:21714 CAPLUS

DOCUMENT NUMBER: 58:21714

ORIGINAL REFERENCE NO.: 58:3633e-f

TITLE: Relations between structure and albumin-binding of amines tested with crossing-paper electrophoresis

AUTHOR(S): Bickel, M. H.; Bovet, D.

CORPORATE SOURCE: Ist. Super. Sanita, Rome

SOURCE: Journal of Chromatography (1962), 8, 466-74  
 CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

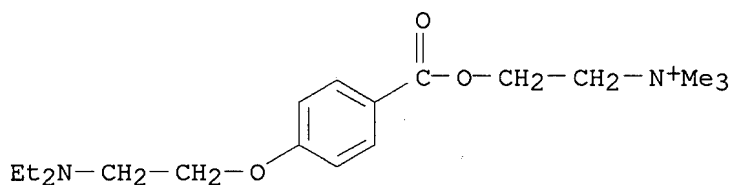
LANGUAGE: Unavailable

AB cf. CA 56, 4041h. A total of 75 N-containing substances was screened with regard to their interaction with blood albumin by means of crossing-paper electrophoresis (loc. cit.). Only tertiary amines with at least 1 substantial radical interact, whereas primary and secondary amines and quaternary NH<sub>4</sub><sup>+</sup> salts do not. With mixed amines, interaction only occurs if the tertiary N dominates the other amino groups.

IT 856619-26-6, Choline, p-[2-(diethylamino)ethoxy]benzoate (ester) (reaction with albumin)

RN 856619-26-6 CAPLUS

CN Choline, p-[2-(diethylamino)ethoxy]benzoate (ester) (7CI) (CA INDEX NAME)



L8 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1963:21330 CAPLUS  
 DOCUMENT NUMBER: 58:21330  
 ORIGINAL REFERENCE NO.: 58:3570c  
 TITLE: Vinyl polymer compositions for dentures  
 INVENTOR(S): Rossetti, Carlo  
 PATENT ASSIGNEE(S): Kulzer & Co. G.m.b.HM.  
 SOURCE: 3 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

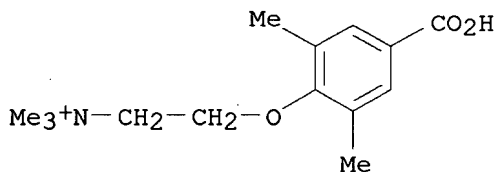
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1138226		19621018	DE 1953-C7820	19530629 <--
PRIORITY APPLN. INFO.:			DE	19530629

AB Polymers suitable for artificial teeth, fillings, etc., are prepared by mixing a vinyl monomer, a powdered polymer, a min. amount of a sulfinic acid, and a quaternary base. Thus, to monomeric Me methacrylate containing 2% benzenesulfinic acid, 0.5% benzyl(diisobutylphenoxyethoxy)-dimethylammonium hydroxide was added. Enough powdered poly(Me methacrylate) was added to make a readily workable paste. Polymerization was complete at 18° after 8 min.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
 (catalysts from sulfinic acids and, in polymerization of Me methacrylate for dentures)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
 (CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1962:456059 CAPLUS  
 DOCUMENT NUMBER: 57:56059  
 ORIGINAL REFERENCE NO.: 57:11115c-f  
 TITLE: Basic substituted alkyl ethers from o-cresotic acid

esters and its salts  
 INVENTOR(S): Hiltmann, Rudolf; Mietzech, F.; Mietzsch, Fritz;  
 Kaemmeter, Kurt  
 SOURCE: 4 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

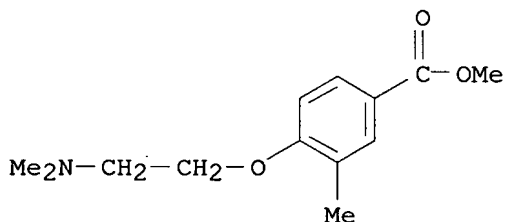
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1118219		19621130	DE 1957-F0022404	19570221 <--
PRIORITY APPLN. INFO.:			DE	19570221

AB Anesthetics for veterinary use with prolonged efficiency are prepared by reaction of o-cresotic acid esters with dialkylaminoalcs, or HORY (R = alkylene with 2 or 3 C atoms, Y = a substituent transformable into mono- or dialkylamino group) in presence of acid binding agents. E.g., 41.5 g. 3,2-Me(HO)C6H3CO2Me is added to 5.8 g. Na in 200 ml. MeOH, distd, in vacuo. Dry residue is suspended in 200 ml. anhyd, toluene, boiled and 30 g. Me2NCH2Cl, diluted with PhMe is dropped in slowly and refluxed 24 hrs. After cooling, the solution is washed with H2O, 2 times with 5% NaOH. After extraction with 2N HCl, base is precipitated with K2CO3 solution, taken up in C6H6, dried, and distilled, giving 30 g. 3,2-Me(Me2NCH2CH2O)C6H3CO2Me, b5 1346°; HCl salt m. 127°. Similarly were prepared: 3,2-Me(Me2NCH2CH2CH2O)C6H3CO2Me, b5 149-52° (HCl salt m. 90-1°); 3,2-Me(Et2NCH2CH2O)C6H3CO2Me, b4 147-9° (HCl salt m. 122°); 3,2-Me(Me2NCH2CH2CH2O)C6H3CO2Et, b4 145-9° (HCl salt m. 143-4°); 3,2-Me(Et2NCH2CH2CH2O)C6H3CO2Et, b3 161-2°; 3,2-Me2NCH2CH2O)C6H3CO2Et, b5 151° phosphate m. 93-5°.

IT 857370-73-1P, m-Toluic acid, 4-[2-(dimethylamino)ethoxy]-, methyl ester, hydrochloride  
 RL: PREP (Preparation)  
 (preparation of)

RN 857370-73-1 CAPLUS

CN m-Toluic acid, 4-[2-(dimethylamino)ethoxy]-, methyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L8 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1962:430619 CAPLUS  
 DOCUMENT NUMBER: 57:30619  
 ORIGINAL REFERENCE NO.: 57:6178c-g  
 TITLE: Antistatic, soft, and microorganism-resistant fabric  
 INVENTOR(S): Sherrill, Joseph C.; Linfield, Warner M.; Marsh, Byron E.  
 PATENT ASSIGNEE(S): Armour & Co.

SOURCE: 5 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3033704		19620508	US 1959-814149	19590519 <--
DE 1195265			DE	
GB 930333			GB	

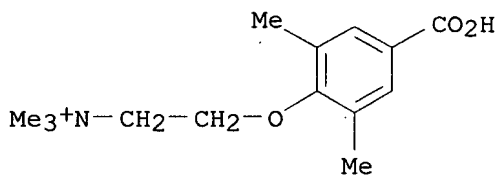
GI For diagram(s), see printed CA Issue.

AB A laundered fabric is impregnated, while rinsing, with one or more cationic surfactants (I) and an organomercurial germicide (II), to render it antistatic, soft and partially free from microorganisms. The fabric is then dried. Three formulas for I are specified:  $[R_1N(R_2)(R_3)_2]^+X^-$  (III),  $[(R_1)_2N(R_2)R_3]^+X^-$  (IV), and V where  $R_1$  is a C10-22 alkyl radical,  $R_2$  is a benzyl radical or an alkyl radical containing <3 C atoms,  $R_3$  is an alkyl radical containing <3 C atoms, and X is chloride, bromide, sulfate, or an alkyl sulfate in which the alkyl radical contains <5 C atoms.  $R_1$  may be a natural mixture derived from tallow, soybean, or coconut oil. III tends toward greater germicidal activity than IV, but the latter has greater softening action and even better results are obtained from III and IV, in which  $R_1$  is a C12-18 alkyl radical,  $R_2$  is a benzyl radical,  $R_3$  a Me radical, and X is chloride. Best results are obtained when II is phenylmercuric acetate, propionate, butyrate, chloride, bromide, or iodide. A typical formulation is 13.7% Softener 2-132 (75%), 10% Arquad S (50%), 0.85% PhHg-OCOC<sub>2</sub>H<sub>5</sub>, 2% hexylene glycol, 0.2% Na<sub>2</sub>SO<sub>4</sub>, 0.5% pigment dye, 0.38% brightener, 0.125% perfume, and H<sub>2</sub>O up to 100%. This is added to the rinse at 12 fl. oz./100 lb. fabric. An example of the efficacy of the treatment is shown, wherein a fabric treated with a concentration of 0.079% of I and 50 p.p.m. II, based on the weight of fabric, shows an average zone of inhibition vs. Staphylococcus aureus of 6 mm. Where treatment takes place in 2 stages, i.e. in a solution of I and then in a solution of II, the zone of inhibition is narrower.

IT 618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
(as cationic surfactant in antistatic, bacteriostatic softening finish for textiles)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
(CA INDEX NAME)

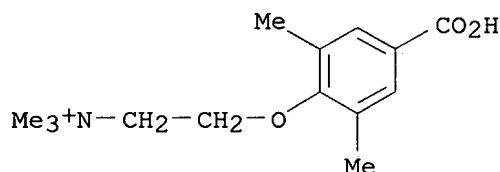


● Cl<sup>-</sup>

L8 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1962:430499 CAPLUS  
DOCUMENT NUMBER: 57:30499  
ORIGINAL REFERENCE NO.: 57:6154d-g

TITLE: Organopolysiloxane foam preparation at room temperature  
 INVENTOR(S): Weyer, Donald E.  
 PATENT ASSIGNEE(S): Dow Corning Corp.  
 SOURCE: 4 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	US 3024210		19620306	US 1959-853697	19591118 <--
AB	A permanent, heat-stable foam, created by rapid evolution of H <sub>2</sub> , is formed at room temperature by mixing an organopolysiloxane, catalyst, and a hydroxylated compound. The organopolysiloxane of the general formula (RHSiO) <sub>x</sub> contains 1-1.8 hydrocarbon radicals per Si which can be either univalent hydrocarbon, halogenated hydrocarbon, or halophenoxymethyl radicals. In addition, the organopolysiloxane contains at least 1% by weight of units with at least 1 H atom attached to Si. Often copolymers or mixts. of homopolymers are used. The catalysts are quaternary ammonium compds. of the type R <sub>4</sub> 'NOH, R <sub>4</sub> 'NOR'', R <sub>4</sub> 'NOCOR''', and R <sub>3</sub> SiONR <sub>4</sub> ' where R', R'', and R''' are mainly aliphatic radicals. The hydroxylated compound can be a low-mol.-weight silanol, H <sub>2</sub> O, or alc. In an example, 100 g. of a copolymer of phenylmethylsiloxane 40, methylhydrogensiloxane 20, monophenylsiloxane 30 and HSiO <sub>3/2</sub> 10 mole % were mixed with 2 g. BuOH and 2 cc. of a 20% solution of benzyl(β-hydroxyethyl)dimethylammonium butoxide. Foaming was complete within 0.5 hr.; foam d. 25 lb./cu. ft.				
IT	618880-92-5, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (catalysts, in foaming of polysiloxanes in presence of hydroxy compds.)				
RN	618880-92-5 CAPLUS				
CN	Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI) (CA INDEX NAME)				



● Cl<sup>-</sup>

L8 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:2737 CAPLUS  
 DOCUMENT NUMBER: 56:2737  
 ORIGINAL REFERENCE NO.: 56:565d-f  
 TITLE: Selective coating of surfaces with organopolysiloxane resins  
 INVENTOR(S): Clark, Harold A.  
 PATENT ASSIGNEE(S): Dow Corning Corp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3002848		19611003	US 1960-669060	19600204 <--

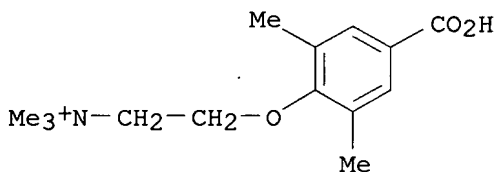
PRIORITY APPLN. INFO.: US 19600204

AB A method is described for selectively coating surfaces with organopolysiloxane resins which gives a sharp delineation between the coated and uncoated portions of the surface and provides an improved way of preparing electronic equipment. Thus, a com. Cu-coated epoxide resin-glass laminate was dipped into a 50% toluene solution of a copolymer of 75 mole % monoethylsiloxane and 25 mole % mono(2-phenylpropyl)siloxane, containing 1.25% by weight Si-bonded OH and 0.15% by weight benzyltrimethylammonium acetate, based on the weight of the copolymer. The coated laminate was dried at room temperature to remove the solvent. A trimethylolethane isophthalate ester (acid number 16) was dissolved in a mixture of BuOAc and EtOH to give a 50% by weight solution of the ester which was applied to various areas of the uncured silicone resin coating on the Cu surface. The BuOAc-EtOH solvent was evapd, at room temperature, and the assembly cured 20 min. at 150°. The laminate was washed with Me Cellosolve which removed the ester coating, with the uncured silicone resin beneath the coating leaving a sharply defined pattern corresponding to the areas covered by the acid ester. The exposed Cu surface was etched with a standard FeCl3-HCl solution which did not affect the Cu under the cured siloxane resin. The cured resin was removed by washing with toluene which exposed a clean Cu surface ready for fabrication of electronic devices.

IT 618880-92-5P, Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride  
 RL: PREP (Preparation)  
 (catalysts, in curing of siloxanes in manufacture of printed elec. circuits)

RN 618880-92-5 CAPLUS

CN Ammonium, [2-[(4-carboxy-2,6-xylyl)oxy]ethyl]trimethyl, chloride (7CI)  
 (CA INDEX NAME)



● Cl<sup>-</sup>

L8 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:40409 CAPLUS

DOCUMENT NUMBER: 52:40409

ORIGINAL REFERENCE NO.: 52:7216b-i,7217a

TITLE: Synthetic curare compounds. VIII. Ether-esters of choline with p-hydroxyaryl- and arylalkylcarboxylic acids

AUTHOR(S): Rosnati, Vittorio

SOURCE: Rend. ist. super. sanita (1955), 18, 998-1013

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB p-IR'3N(CH2)2O2CC6H4O(CH2)nNR3I (I), p-IR'3(CH2)2O2CCH2C6H4O(CH2)nNR3I (II), and p-IR'3N(CH2)2O2CCH2CH2C6H4O(CH2)nNR3I (III) were prepared, n = 2

or 3, and R, R' = Me or Et. Several of the intermediates prepared were new. I were prepared in fair to good yields through the following steps. Et p-hydroxybenzoate in absolute EtOH containing Na refluxed with Cl(CH<sub>2</sub>)<sub>n</sub>NR<sub>2</sub>,

NaCl

filtered off, the filtrate evaporated, extracted with Et<sub>2</sub>O, and distilled gave p-R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et (IV). So obtained were IV (R = Me, n = 3), b0.05 119-20°, and IV (R = Et, n = 3), b0.06 128-9°. From IV, the intermediate p-R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>OC<sub>6</sub>H<sub>4</sub>.CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>NR'<sub>2</sub> (V) resulted by transesterification with excess HO(CH<sub>2</sub>)<sub>2</sub>NR<sub>2</sub> and a small amount of Na, or in the case of IV (R = Me, n = 3) (which failed to react) by saponifying the Et ester to the free acid, treating the dried acid with PCl<sub>5</sub> to form HCl.Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>COCl, which was in turn reacted with excess HO(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub> in CHCl<sub>3</sub> to form V (R, R' = Me, n = 3), b0.07 146-9°, V (R = Et, R' = Me, n = 3), b0.06 133-4°, V (R, R' = Et, n = 3), b0.05 152-4°. These were treated with MeI or EtI to form I: R<sub>3</sub>, R'<sub>3</sub> = Me<sub>3</sub>, n = 3 (VI), m. 262-4°; R<sub>3</sub> = Et<sub>2</sub>Me, R'<sub>3</sub> = Me<sub>3</sub> (VII), m. 227-8°; R<sub>3</sub>, R'<sub>3</sub> = Et<sub>3</sub> (VIII), m. 197-9°. II were similarly prepared from p-hydroxyphenylacetic acid through p-R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>Et (IX): R = Et, n = 2, b0.06 116-18°; R = Me, n = 3, b0.05 113-14°; R = Et, n = 3, b0.06 132°. From IX, further reaction with HO(CH<sub>2</sub>)<sub>n</sub>NR<sub>2</sub> yielded p-R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>NR'<sub>2</sub> (X): R, R' = Et, n = 2, b0.06 142-5°; R, R' = Me, n = 3, b0.06 127-9°; R = Et, R' = Me, n = 3, b0.06 159-60°; R, R' = Et, n = 3, b0.06 162-3°. X with MeI or EtI yielded II in fair to good yields: R<sub>3</sub>, R'<sub>3</sub> = Et<sub>3</sub>, n = 2 (XI), viscous oil; R<sub>3</sub>, R'<sub>3</sub> = Me<sub>3</sub>, n = 3 (XII), m. 142-4°; R<sub>3</sub> = Et<sub>2</sub>Me, R'<sub>3</sub> = Me<sub>3</sub> (XIII), viscous oil; R<sub>3</sub>, R'<sub>3</sub> = Et<sub>3</sub> (XIV), viscous oil. III (R<sub>3</sub>, R'<sub>3</sub> = Et<sub>3</sub>) (XV), m. 159°, was prepared from 3-(p-hydroxyphenyl)propionic acid via p-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>Et, b0.5 150-2°, and p-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>, b0.07 174-6°. Among the curarizing agents tested, XII and XIII were not effective (at 0.05 mg./kg.), gave action of very brief duration, and were relatively low in toxicity. VI and VII were also quite effective (at 0.2 mg./kg.) with a more prolonged action similar to that of Flaxedil. The others (VIII, XI, XIV, XV) were less effective, with XIV and XV lowest in toxicity. Other compds. prepared were: p-MeO<sub>2</sub>CCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me, m. 96-8°, by refluxing 30 g. p-carboxyphenoxyacetic acid (XVI) (cf. Christiansen, C.A. 19, 1417) with 150 ml. MeOH saturated with HCl 7 hrs., filtering, and crystallizing the

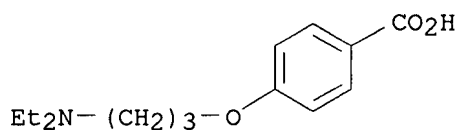
solution

on ice (yield 22.5 g.). p-ClOCCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>COCl (XVII), b0.08 107-8°, was prepared from 20 g. XVI by adding 40 g. PCl<sub>5</sub> in small portions, allowing the reaction to subside, refluxing 1 hr., extracting the material with C<sub>6</sub>H<sub>6</sub>, and distilling p-Me<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>OCCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub> (XVIII), b0.05 160-78°, was prepared in 6.6 g. yield by dissolving 10 g. HO(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub> in 150 ml. CHCl<sub>3</sub>, saturating the solution with HCl gas, adding 8 g. XVII in 60 ml. CHCl<sub>3</sub>, refluxing 6 hrs., cooling, adding 50 ml. ice H<sub>2</sub>O, acidifying with 1:1 HCl, removing the CHCl<sub>3</sub> phase, neutralizing the aqueous phase with K<sub>2</sub>CO<sub>3</sub>, and extracting with Et<sub>2</sub>O. XVIII with MeI yielded IMe<sub>3</sub>N(CH<sub>2</sub>)<sub>2</sub>OCCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>NMe<sub>3</sub>I, m. 231-3°. The Et analog of XVIII, b0.06 171-3°, was made in a similar way, but reaction with EtI yielded p-IEt<sub>3</sub>N(CH<sub>2</sub>)<sub>2</sub>OCCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, m. 149-51°, which crystallized by slowly adding Et<sub>2</sub>O to the cold EtOH solution. Dimethylaminoethyl phenoxyacetate, b0.6 109-10°, its Et analog, b0.4 115-16°, and the respective quaternary compds., m. 147°, and m. 140-1°, were prepared in similar fashion from ClOCCH<sub>2</sub>OPh and the HCl salt of the amino alc.

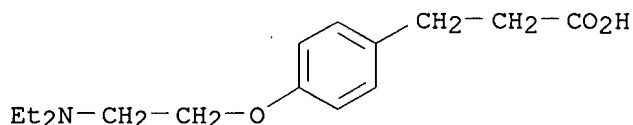
IT

551935-15-0, Benzoic acid, p-(3-diethylaminopropoxy)-  
556639-07-1, Hydrocinnamic acid, p-(2-diethylaminoethoxy)-  
857169-86-9, Acetic acid, [p-(3-dimethylaminopropoxy)  
phenyl]- 857170-47-9, Acetic acid, [p-(3-diethylaminopropoxy)phenyl]-  
(derivs.)

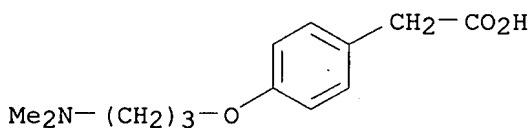
RN 551935-15-0 CAPLUS  
CN Benzoic acid, 4-[3-(diethylamino)propoxy]- (CA INDEX NAME)



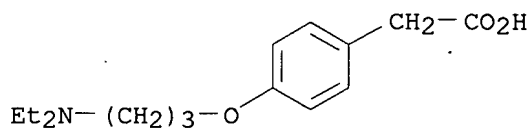
RN 856639-07-1 CAPLUS  
CN Hydrocinnamic acid, p-(2-diethylaminoethoxy)- (6CI) (CA INDEX NAME)



RN 857169-86-9 CAPLUS  
CN Acetic acid, [p-(3-dimethylaminopropoxy)phenyl]- (6CI) (CA INDEX NAME)



RN 857170-47-9 CAPLUS  
CN Acetic acid, [p-(3-diethylaminopropoxy)phenyl]- (6CI) (CA INDEX NAME)



L8 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:6242 CAPLUS

DOCUMENT NUMBER: 52:6242

ORIGINAL REFERENCE NO.: 52:1101a-f

TITLE: Synthetic curare compounds. IX. Ether-esters of choline with p-hydroxyphenyl-substituted carboxylic acids

AUTHOR(S): Rosnati, Vittorio; Puschner, Heinz

CORPORATE SOURCE: Ist. super. Sanita, Rome

SOURCE: Gazzetta Chimica Italiana (1957), 87, 586-96

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

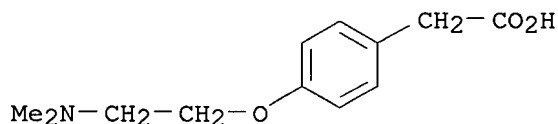
AB cf. C.A. 47, 7437c. To 27.5 g. NaOH in 360 cc. H<sub>2</sub>O is added 54 g. p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H (I), 250 g. (BrCH<sub>2</sub>)<sub>2</sub>, and 750 cc. 95% EtOH, the mixture refluxed 1 hr., 3 g. NaOH added, refluxing continued 1 hr., the solvent stripped in vacuo, the residue dissolved in 300 cc. H<sub>2</sub>O and 100 cc. EtOH, and acidified with diluted H<sub>2</sub>SO<sub>4</sub>, yielding 50 g. crude product consisting mainly of p-(2-bromoethoxyphenyl)acetic acid (II), m. 108-10° (Me ester, b<sub>0.2</sub> 128-9°), and some glycol diether of I (III), m. 249-50°; di Me ester, m. 128-9°. III is separated from II by

the insoly. of the diester in MeOH. II (15 g.) and 150 cc. 20% aqueous NHMe<sub>2</sub> is heated to 110° 5 hrs., evaporated to dryness, dissolved in 200 cc. absolute EtOH, saturated with HCl gas, and refluxed 4 hrs., the product evaporated, the residue dissolved in 30 cc. H<sub>2</sub>O, filtered, washed with Et<sub>2</sub>O, made alkaline, and repeatedly extracted with Et<sub>2</sub>O, and the exts. dried and distilled giving 8 g. Et p-(2-diethylaminoethoxyphenyl)acetate (IV), b0.2 130°; picrate, m. 116-18°. (An alternate method of preparation of IV is the condensation of I Et ester with 1-dimethylamino-2-chloroethane.) IV (8 g.) is added to 0.05 g. Na in 40 cc. 2-dimethylaminoethanol (V) and the mixture slowly distilled 1 hr. through an efficient column, 20 cc. V and 0.05 g. Na added, the distillation resumed, and the distillates stripped of V, dissolved in Et<sub>2</sub>O, washed with H<sub>2</sub>O, and fractionated, yielding 6 g. 2-dimethylaminoethyl ester of p-(2-dimethylaminoethoxy)phenylacetic acid, b0.05 130°; bisiodomethylate (VI), m. 146-8°. The phenylpropionic acid derivs. were prepared analogously, giving 3-(p-2-bromomethoxyphenyl)propionic acid, m. 131-2° (Me ester, m. 53-4°); glycol ether of 3-(p-hydroxyphenyl)propionic acid, m. 233-4° (Me ester, m. 166-7°); 3-(p-2-dimethylaminoethoxyphenyl)propionic acid (VII), m. 140-1° (Et ester, b0.1 146°); 2-dimethylaminoethyl ester of VII, b0.06 134-5° [bisiodomethylate (VIII), m. 165-6°]. According to an alternate route of synthesis, p-hydroxycinnamic acid is hydrogenated to the p-glycol monoether of phenylpropionic acid, m. 109-11°, converted to 3-(p-2-chloroethoxyphenyl)propionic acid (IX), m. 123-4°, and subsequently to 2-dimethylaminoethyl ester of IX, b0.05 175-80°. The curarelike activity of VI and VIII is strong and of short duration.

IT 857170-02-6, Acetic acid, [p-(2-dimethylaminoethoxy)phenyl]  
 ]-  
 (derivs.)

RN 857170-02-6 CAPLUS

CN Acetic acid, [p-(2-dimethylaminoethoxy)phenyl]- (6CI) (CA INDEX NAME)



L8 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1957:71492 CAPLUS

DOCUMENT NUMBER: 51:71492

ORIGINAL REFERENCE NO.: 51:12915b-i,12916a-i,12917a

TITLE: Derivatives of 4-amino-2-hydroxybenzoic acid. V. Basic ethers

AUTHOR(S): Clinton, R. O.; Laskowski, S. C.; Salvador, U. J.; Carroll, Patricia M.

CORPORATE SOURCE: Sterling-Winthrop Research Inst., Rensselaer, NY

SOURCE: Journal of the American Chemical Society (1957), 79, 2290-5  
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 51:71492

AB 2,4-HO(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Me (39.4 g.) in 1400 cc. dry PhMe treated with 4.6 g. Na and 500 cc. absolute MeOH, the MeOH distilled with stirring up to 110°, the residual suspension refluxed 20 hrs. with stirring with 29.8 g. Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>Cl in 500 cc. dry PhMe, cooled, and filtered, the filter residue

washed with dry C<sub>6</sub>H<sub>6</sub>, the combined filtrate and washing evaporated in vacuo, and the oily residue treated in EtOAc with excess dry HCl in Et<sub>2</sub>O yielded 85% 2,4-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Me.HCl. m. 156.9-9.2°; picrate, m. 149.8-50.6° (all m.ps. are corrected). 2,4-HO(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Pr (24.7 g.), 16.3 g. Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>Cl, and 250 cc. PrOH refluxed 8 hrs. with stirring gave after the usual procedure 1.0 g. 2,4-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Pr.HCl, m. 153.4-5.4°; picrate, m. 98.8-100.6°. 2,4-HO(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et treated in the usual manner with p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>Cl gave 2,4-ClCH<sub>2</sub>CH<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et, pale yellow platelets, 56.6-7.2°, which refluxed with a secondary amine in EtOH with NaI yielded 50-65% dialkylamino derivative. The appropriate alkyl 2-hydroxy-4-nitrobenzoate, Na alkoxide, and dialkylaminoalkyl chloride under anhydrous conditions gave by the general procedure described previously (C.A. 48, 5852h) the corresponding 2,4-R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>R'.HCl (I); in runs with Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>Cl using the appropriate alc. as the reaction medium were obtained the following I with R = Et in the yields indicated (R' given): Me in MeOH, 5; Et in EtOH, 71; Pr in PrOH, 88; Bu in BuOH, 86; Et in EtOH from Me ester, 70. By the methods described were prepared the following I (R<sub>2</sub>N, R', n, m.p., and m.p. of picrate given): Me<sub>2</sub>N, Et, 2, 202.2-2.6°, 139.4-40.4°; Et<sub>2</sub>N, Et, 2, 143.9-4.8°, 137.8-9.0°; Et<sub>2</sub>N, Bu, 2, 117.6-18.6°, 120.5-1.6°; Et<sub>2</sub>N, Et, 3, 164.8-5.6°, 98.6-9.2°; iso-Pr<sub>2</sub>N, Et, 2, 169.1-70.7°, 160.3-3.2° (base, m. 42.0-8.9°); morpholino, Me, 2, 206.0-6.4°, 161.6-2.2°; morpholino, Et, 2, 207.0-8.0°, 154.8-5.6°; morpholino, Et, 3, 142.0-4.6°, 133.4-4.2°; 1-piperidyl, Et, 2, 191.0-1.5°, 141.7-2.9°; 1-piperidyl, Et, 3, 160.4-1.6°, 139.6-140.4°; 2-methyl-1-piperidyl, Et, 2, 180.8-2.6°, 138.0-9.0°; 2-methyl-1-piperidyl, Et, 3, 158.2-9.6°, 104.6-8.8°; 2,6-dimethyl-1-piperidyl, Et, 2, 153.0-4.0°, 207.6-9.0°. The appropriate I in EtOAc treated under anhydrous conditions with 3 moles MeI or MeBr, kept 3-20 hrs. at room temperature, and filtered gave the corresponding quaternary salt; the I in MeCN refluxed 36-72 hrs. with 3 moles of the appropriate alkyl bromide gave the corresponding salt. In this manner were prepared the following 2,5-EtO<sub>2</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>.RBr (R, and m.p. given): Me, - (iodide, m. 190.2-1.2°); Et, - (iodide, m. 119.1-20.2°); iso-Pr, 180.1-2.4°; iso-Bu, 137.4-8.2°; iso-Am, 150.6-3.0°; HOCH<sub>2</sub>CH<sub>2</sub>, 129.7-38.0°; PhCH<sub>2</sub>, 153.3-5.1°; 2-cyclohexylethyl, 121.9-3.5°. [2,5-EtO<sub>2</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>]<sub>2</sub>.(CH<sub>2</sub>)<sub>n</sub>Br<sub>2</sub> (n and m.p. given): 2, 164.1-72.0°; 3, 185.1-92.0°; 4, 179.0-86.9°; 5, 184-7° (decomposition) with sintering from 152° when immersed at 25°; 6, 192.3-5.9°. 2,5-RO<sub>2</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>.MeI (R, and m.p. given): Me, 162.5-3.0°; Et, 143.1-4.6° (bromide, m. 150.6-1.6°); Pr, 143.2-4.6°; Bu, 118.2-20.3°. [2,5-EtO<sub>2</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>]<sub>2</sub>.(CH<sub>2</sub>)<sub>n</sub>Br<sub>2</sub> (n and m.p. given): 2, 146.7-8.7°; 4, 143.2-6.8°; 6, 150.7-8.2°. 2,5-R'O<sub>2</sub>C(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>n</sub>NR<sub>2</sub>.R''X (R<sub>2</sub>N, R', R'', n, X, and m.p. given): Et<sub>2</sub>N, Et, Et, I, 2, 140.7-1.9°; Et<sub>2</sub>N, Et, Me, I, 3, 149.0-9.6°; iso-Pr<sub>2</sub>N, Et, Me, I, 2, 183.7-4.2°; morpholino, Me, Me, I, 2, 209.0-11.0°; morpholino, Et, Me, I, 2, 190.5-1.3°; morpholino, Et, Me, I, 3, 161.1-1.7°; 1-piperidyl, Et, Me, I, 2, 147.7-8.9°; 1-piperidyl, Et, Me, I, 3, 166.9-7.9°; 2-methyl-1-piperidyl, Et, Me, I, 2, 159.8-61.0°; 2-methyl-1-piperidyl, Et, Me, I, 3, 165.5-6.5°; 2,6-dimethyl-1-piperidyl, Et, Me, I, 2, 192.3-2.9°. The appropriate alkyl 2-(dialkylaminoalkoxy)-4-nitrobenzoate (0.01 mole) and 0.02 mole 2,4-HO(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CN in EtOAc yielded essentially quantitatively the corresponding alkyl 2-(dialkylaminoalkoxy)-4-nitrobenzoate 2-cyano-5-nitrophenolate (alkyl, dialkylaminoalkoxy group, crystal form, and m.p. given): Et, Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O, canary-yellow prisms, 76.0-8.0°;

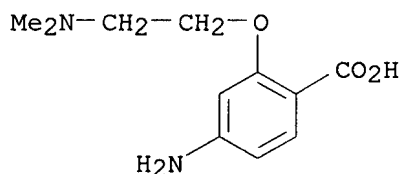
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Et, 3-piperidinopropoxy, short blunt orange needles, 125.2-6.0°;  
Et, 3-morpholinopropoxy, hair-like yellow-orange needles,  
137.2-8.3°. 2,4-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et.HCl (15.0 g.), 18.3 g.  
Na<sub>2</sub>CO<sub>3</sub>, and 200 cc. 50% EtOH refluxed 4 hrs. with stirring, the EtOH  
removed in vacuo, the aqueous residue acidified with concentrated HCl to Congo

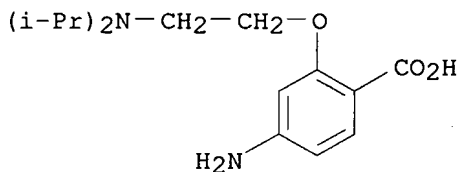
and saturated with (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, and the precipitate filtered off yielded 13.8 g.  
2,4-Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>H (II) HCl salt, m. 212.5-13.9° (from  
MeOH). II.HCl (31.9 g.), 8.4 g. NaHCO<sub>3</sub>, and 500 cc. absolute EtOH refluxed 3  
hrs. with stirring, cooled, filtered, and evaporated in vacuo gave 25.0 g. II,  
m. 164.6-6.6°; picrate, cottony yellow needles, m.  
179.2-80.4°. Similarly was prepared 2,4-Me<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>H,  
cream-colored plates, m. 193.1-4.1° (from absolute EtOH) [HCl salt,  
pale yellow needles, m. 208.0-9.6° (from absolute EtOH); picrate,  
clusters of yellow needles, m. 181.8-2.6°], and  
2-(3-piperidinopropoxy)-4-nitrobenzoic acid HCl salt, pale yellow cotton  
needles, m. 216.8-17.5° (from absolute EtOH) [picrate, canary-yellow  
needles, m. 143.0-5.0° (from absolute EtOH)]. The appropriate alkyl  
2-(dialkylaminoalkoxy)-4-nitrobenzoate base or HCl salt reduced in the  
appropriate dilute alc. with Fe and HCl or catalytically at 25° in  
the appropriate alc. over PtO<sub>2</sub> gave the corresponding 4,2-  
H<sub>2</sub>N[R<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>O]C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>R' (R<sub>2</sub>N, R', m.p. of phosphate, and m.p. of picrate  
given). With n = 2: Me<sub>2</sub>N, Et, 176.3-7.3°, 140.2-1.2° (base,  
m. 94.2-5.6°); Et<sub>2</sub>N, Me, 195.8-6.8°, 119.0-20.4°  
(dipicrate); Et<sub>2</sub>N, Et, 168.7-9.6°, 131.6-3.2° (di-HCl salt,  
m. 173.6-3.9°); Et<sub>2</sub>N, Pr, 153.0-4.0°, 140.4-1.2°;  
Et<sub>2</sub>N, Bu, 154.5-5.5°, 120.8-2.6°; iso-Pr<sub>2</sub>N, Et,  
186.0-7.0°, -(flavinate, m. 196.8-7.8°); morpholino, Me,  
151.3-2.1° (diphosphate), 168.5-9.7°; morpholino, Et,  
196.3-6.9°, 165.8-6.8° (base, m. 98.0-9.8°);  
piperidino, Et, 220.8-1.4°, 159.0-60.0° (base, m.  
107.3-8.5°); 2-methylpiperidino, Et, -, 172.4-3.6° (base, m.  
91.2-2.4°); 2,6-dimethylpiperidino, Et, 211.0-11.8°,  
188.8-9.6°. With n = 3: Et<sub>2</sub>N, Et, 151.5-3.2°,  
146.2-7.0°; morpholino, Et, 143.3-4.4°, 210.4-11.4°  
(base, m. 106.8-8.0°); piperidino, Et, 160.2-1.6°,  
218.0-18.7° (base, 109.2-10.1°); 2-methylpiperidino, Et,  
136.4-8.3°, 180.8-3.0° (base, m. 112.4-13.8°). The  
appropriate alkyl 2-(dialkylaminoalkoxy)-4-nitrobenzoate quaternary and  
bisquaternary salts gave similarly by Fe-HCl or catalytic reduction the  
4-NH<sub>2</sub> analogs. In this manner were prepared 5,2-  
H<sub>2</sub>N(R'O<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>n</sub>NR<sub>2</sub>.R''X (R<sub>2</sub>N, R', R'', X, and m.p. given). With n =  
2: Me<sub>2</sub>N, Et, Me, I, 204.2-5.2°; Me<sub>2</sub>N, Et, Et, I, 172.3-5.3°;  
Me<sub>2</sub>N, Et, iso-Pr, Br, 190.0-2.2°; Me<sub>2</sub>N, Et, HOCH<sub>2</sub>CH<sub>2</sub>, Br,  
138.9-42.3°; Me<sub>2</sub>N, Et, 2-cyclohexylethyl, Br, 101.6-5.1°;  
Me<sub>2</sub>N, Et, (CH<sub>2</sub>)<sub>2</sub>, Br, 190.0-95° (decomposition); Me<sub>2</sub>N, Et, (CH<sub>2</sub>)<sub>4</sub>, Br,  
150° (indefinite above 160° with decomposition); Me<sub>2</sub>N, Et,  
(CH<sub>2</sub>)<sub>5</sub>, Br, 125° (indefinite above 190° with decomposition);  
Me<sub>2</sub>N, Et, (CH<sub>2</sub>)<sub>6</sub>, Br, 200.7-2.5°; Et<sub>2</sub>N, Me, Me, I,  
127.4-9.0°; Et<sub>2</sub>N, Et, Me, Br, 160.3-2.1°; Et<sub>2</sub>N, Et, Me, I,  
139.2-41.1°; Et<sub>2</sub>N, Pr, Me, I, 127.4-9.6°; Et<sub>2</sub>N, Bu, Me, I,  
88.2-92.4°; Et<sub>2</sub>N, Et, Et, I, 141.2-3.8°; morpholino, Et, Me,  
I, 182.7-3.7°; piperidino, Et, Me, I, 167.4-8.4°;  
2,6-dimethylpiperidino, Et, Me, I, 123.4-6.4°. With n = 3: Et<sub>2</sub>N,  
Et, Me, I, 125.0-6.0°; morpholino, Br, Me, I, 151.9-3.1°;  
piperidino, Et, Me, I, 150.1-50.6°. The appropriate  
2-(dialkylaminoalkoxy)-4-nitrobenzoic acids or their HCl salts reduced  
catalytically yielded the corresponding 4-amino-2-(2-  
dialkylaminoalkoxy)benzoic acids (dialkylaminoalkoxy group, crystal form,  
arid m.p. given): Et<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O, needles, 158.0-8.8° (decomposition)  
[picrate, canary-yellow needles, m. 187.5-8.3° (from EtOH)];  
Me<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>O, -, -(HCl salt, needles, m. 145.5-7.2° with decomposition);

3-piperidinopropoxy, -, -(HCl salt, tan needles, m. 162.1-2.8° with decomposition). Reductive alkylation of the appropriate 4-NH<sub>2</sub> bases with an aldehyde, Zn dust, and AcOH gave 4,2-BuNH(Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>O)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et.HCl, cream-colored needles, m. 160.5-1.8° (from absolute EtOH-EtOAc) [flavianate, yellow-orange plates, m. 164.6-5.6° (from EtOH)], 4,2-HO(CH<sub>2</sub>)<sub>5</sub>NH(Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>O)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et.HCl, cottony needles, m. 132.2-3.4° (from absolute EtOH hexane) (flavianate, cottony orange needles, m. 126.0-6.4°), Et 4-(2,2-dimethyl-3-hydroxypropylamino)-2-[2-(2,6-dimethylpiperidino)ethoxy] benzoate, needles, m. 90.0-1.0° (from C<sub>6</sub>H<sub>6</sub>).

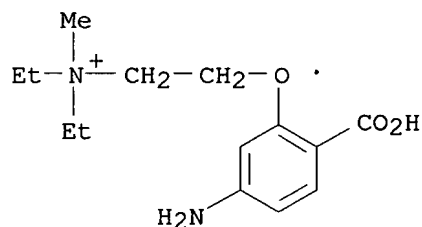
IT 807293-69-2, Benzoic acid, 4-amino-2-(2-dimethylaminoethoxy)-  
856788-92-6, Benzoic acid, 4-amino-2-(2-diisopropylaminoethoxy)-  
(derivs.)  
RN 807293-69-2 CAPLUS  
CN Benzoic acid, 4-amino-2-[2-(dimethylamino)ethoxy]- (CA INDEX NAME)



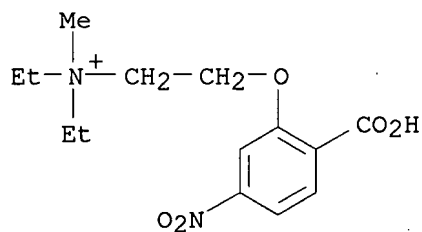
RN 856788-92-6 CAPLUS  
CN Benzoic acid, 4-amino-2-(2-diisopropylaminoethoxy)- (6CI) (CA INDEX NAME)



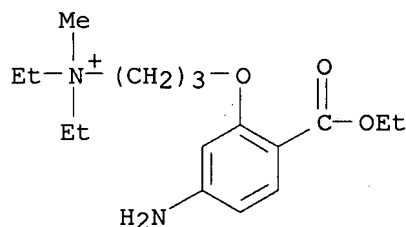
IT 857174-71-1, Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]diethylmethyl-  
ethyl- 857179-13-6, Ammonium, [2-(2-carboxy-5-nitrophenoxy)ethyl]diethylmethyl-  
(halides, esters)  
RN 857174-71-1 CAPLUS  
CN Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]diethylmethyl- (6CI) (CA INDEX NAME)



RN 857179-13-6 CAPLUS  
CN Ammonium, [2-(2-carboxy-5-nitrophenoxy)ethyl]diethylmethyl- (6CI) (CA INDEX NAME)

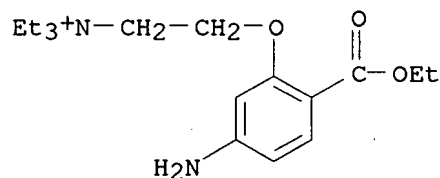


IT 857174-47-1P, Ammonium, [3-(5-amino-2-carboxyphenoxy)propyl]diethylmethyl-, iodide, Et ester  
 857174-56-2P, Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]triethyl-, iodide, Et ester 857174-64-2P,  
 Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]ethyldimethyl-, iodide, Et ester  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 857174-47-1 CAPLUS  
 CN Ammonium, [3-(5-amino-2-carboxyphenoxy)propyl]diethylmethyl-, iodide, Et ester (6CI) (CA INDEX NAME)



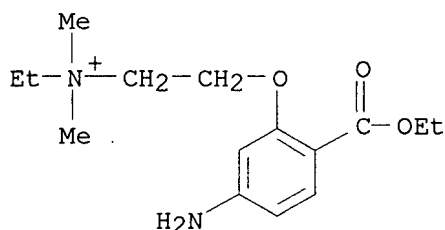
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RN 857174-56-2 CAPLUS  
 CN Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]triethyl-, iodide, Et ester (6CI) (CA INDEX NAME)



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RN 857174-64-2 CAPLUS  
 CN Ammonium, [2-(5-amino-2-carboxyphenoxy)ethyl]ethyldimethyl-, iodide, Et ester (6CI) (CA INDEX NAME)



● I-

L8 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1956:69464 CAPLUS

DOCUMENT NUMBER: 50:69464

ORIGINAL REFERENCE NO.: 50:13044d-h

TITLE: Aryl ketones and thio morpholides in the synthesis of 8-substituted xanthenes

AUTHOR(S): Hager, Geo. P.; Kramer, Stanley P.

CORPORATE SOURCE: Univ. of Maryland, Baltimore

SOURCE: Journal of the American Pharmaceutical Association (1912-1977) (1955), 44, 649-53  
CODEN: JPHAA3; ISSN: 0003-0465

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

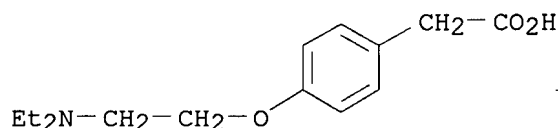
AB The following 8-substituted benzyltheophyllines were prepared by heating equimolar amts. of the appropriate phenylacetic acid and 1,3-dimethyl-5,6-diaminouracil (I) just above the m.p. until the mixture resolidified, dissolving the product in boiling 5% NaOH, precipitating with CO<sub>2</sub>,

and recrystg. from HOAc, absolute EtOH, HCONMe<sub>2</sub>, or mixts. of HOAc with H<sub>2</sub>O, EtOH or Et<sub>2</sub>O. The following compds. were prepared, 8-benzyl substituent and m.p. given: m-HO, above 300°; p-HO, above 300°; 3,4-(HO)<sub>2</sub>, above 300°; m-MeO, 251-2°; p-MeO, 276.7-7.5°; p-EtO, 256°; p-PhCH<sub>2</sub>O, 235.5-57°; p-Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>O, 189.5-90°; 3,4-(MeO)<sub>2</sub>, 246-7°; 3,4-CH<sub>2</sub>O<sub>2</sub>, above 300°; α-MeO, 193.5-4°. 8-Benzyltheophylline, m. 297-8°, was prepared in 32% yield by heating I and phenylthioacetomorpholide 7 hrs. at 110-75°. 4-Aminophenylthioacetomorpholide gave 5% 8-(4-aminobenzyl)theophylline, m. 297-8°. From 7.2 g. PhAc, 2.4 g. S, and 5.1 g. I refluxed 30 min. at 155-70° and 6 hrs. at 170° and worked up as above was obtained 30% 8-benzyltheophylline, m. 276-8°. Substitution of styrene or trithioacetophenone for PhAc in the above reaction gave little or no product. Ethylenediamine-p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H, S, and PhAc in 10 hrs. at 170-85° gave after treatment with HCl in absolute EtOH 3.7% of "2-benzyl-2-imidazolinium chloride," m. 171-3°. p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>Et (22.5 g.), 44 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl.HCl, 138 g. K<sub>2</sub>CO<sub>3</sub>, and 754 ml. dry Me<sub>2</sub>CO refluxed 14 hrs. gave 20 g. p-Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>Et (II), b<sub>2</sub> 155-64°; HCl salt, m. 131.5-2.5°. II (6 g.), 5 ml. HCl, and 40 ml. H<sub>2</sub>O refluxed 8 hrs., evaporated and the residue recrystd. from Me<sub>2</sub>CO gave 5.5 g. p-Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H.HCl, m. 127-8.5°. p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H (15.2 g.) added to 13.6 g. NaOEt in 75 ml. absolute EtOH, the solvent removed in vacuo and the residue refluxed 5 hrs. with 125 ml. HCONMe<sub>2</sub> and 67.8 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl gave 10% p-Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, b<sub>2</sub> 190-211°; di-HCl salt, m. 158-9°.

IT 802559-45-1, Acetic acid, [p-(2-diethylaminoethoxy)phenyl]-  
]-

(derivs.)

RN 802559-45-1 CAPLUS  
CN Acetic acid, [p-[2-(diethylamino)ethoxy]phenyl]- (8CI) (CA INDEX NAME)

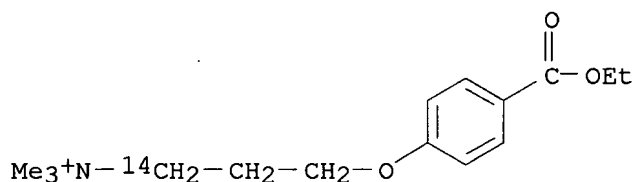


L8 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1956:48568 CAPLUS  
DOCUMENT NUMBER: 50:48568  
ORIGINAL REFERENCE NO.: 50:9321c-i  
TITLE: The o-Claisen transfer. Experiments with carbon-14.  
VII. Also Claisen rearrangements. V. The ortho-Claisen  
rearrangement  
AUTHOR(S): Fahrni, P.; Haegele, W.; Schmid, K.; Schmid, H.  
CORPORATE SOURCE: Univ. Zurich, Switz.  
SOURCE: Helvetica Chimica Acta (1955), 38, 783-9  
CODEN: HCACAV; ISSN: 0018-019X  
DOCUMENT TYPE: Journal  
LANGUAGE: German

AB The ortho-Claisen rearrangement of 2,4-disubstituted Ph allyl ethers (I), contrary to that of 2-monosubstituted I (II), is uniform. II normally form the 6-allyl-2-substituted phenols but also 4-allyl-2-substituted phenols. The exact reaction was proven with 4,2-Me(CH<sub>2</sub>:CHC<sup>14</sup>HCH<sub>2</sub>)C<sub>6</sub>H<sub>3</sub>O:CH<sub>2</sub>CH:CH<sub>2</sub> (III) and 4,2-MeO<sub>2</sub>C(CH<sub>2</sub>:CHC<sup>14</sup>HCH<sub>2</sub>)C<sub>6</sub>H<sub>3</sub>OCH<sub>2</sub>:CHCH<sub>2</sub> (IV). It was investigated if the intermediates in the transfer of III were 2,2-diallyl-4-methyl-3,4-cyclohexadien-1-one and 2,4-diallyl-4-methyl-2,5-cyclohexadien-1-one. A 2,6-diallylphenol free of C<sup>14</sup>H<sub>2</sub>:CHCH<sub>2</sub> was obtained. CICH<sub>2</sub>CH<sub>2</sub>C<sup>14</sup>H<sub>2</sub>OH (7.54 g.) and 14.65 g. 4-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et refluxed 100 hrs. in 40 cc. Me<sub>2</sub>CO with 26.5 g. pulverized KI and 13.2 g. K<sub>2</sub>CO<sub>3</sub>, the cooled mixture treated with H<sub>2</sub>O, extracted with Et<sub>2</sub>O, and the extract washed with H<sub>2</sub>O, 2% NaOH, and brine, dried, and evaporated yielded 12.55 g. (70%) p-EtO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>CH<sub>2</sub>C<sup>14</sup>H<sub>2</sub>OH (V) m. 40.5-1.5° (from Et<sub>2</sub>O:CH<sub>2</sub>Cl<sub>2</sub>). The purest SOCl<sub>2</sub> (6.78 g.) in 13 cc. CHCl<sub>3</sub> added dropwise to 8.483 g. V in 26 cc. CHCl<sub>3</sub> and 3.2999 g. pyridine, the mixture kept 2 hrs. in the dark, then boiled 45 min., and the Cl compound separated in the usual manner, converted into the iodo compound with NaI in Me<sub>2</sub>CO, and finally treated with a 4-fold amount of NMe<sub>3</sub> in alc. yielded 11.9 g. p-EtO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>CH<sub>2</sub>C<sup>14</sup>H<sub>2</sub>NMe<sub>3</sub>I, m. 172.5-4°; 22.03 g. of this compound stirred 48 hrs. in a vibro-mixer with 30 g. AgNO<sub>3</sub> in H<sub>2</sub>O, the mixture filtered, the filtrate evaporated to 50° in vacuo, the crystalline residue heated 16 hrs. to 110-20° with 240 cc. 33% NaOH, 50 cc. H<sub>2</sub>O added, the mixture heated 10 hrs. to 110-20°, cooled, acidified with 1:1 HCl, left overnight, filtered through glass wool, and the filter and filter cake extracted with Et<sub>2</sub>O in a Soxhlet yielded 7.67 g. 4-C<sup>14</sup>H<sub>2</sub>:CHCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, m. 158-60° (from alc.); its Me ester (made with N<sub>2</sub>CH<sub>2</sub>), (4.606 g.) heated 20 hrs. with 9 cc. Et<sub>2</sub>NPh under a high vacuum in a boiling BzMe bath, the product dissolved in Et<sub>2</sub>O, and the extract washed and distilled (b<sub>0.05</sub> 80-100°) gave 3.45 g. 2,4-C<sup>14</sup>H<sub>2</sub>:CHCH<sub>2</sub>(MeO<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>OH, (VI), m. 92-3° (from CCl<sub>4</sub> and Et<sub>2</sub>O-C<sub>5</sub>H<sub>12</sub>), which with MeI and K<sub>2</sub>CO<sub>3</sub> in Me<sub>2</sub>CO yielded 2,4-C<sup>14</sup>H<sub>2</sub>:CHCH<sub>2</sub>(MeO<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>OMe (VII), b<sub>0.05</sub> 125-35°, colorless oil. VII treated in known manner with OsO<sub>4</sub> in pyridine gave 2,4-C<sup>14</sup>H<sub>2</sub>(OH)CH(OH)CH<sub>2</sub>(MeO<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>OMe, m. 173-5° (from AcOEt). VI (2.384 g.) in 9.5 cc. MeOH, and 0.28 g. Na treated with 1.67 g. CH<sub>2</sub>:CHCH<sub>2</sub>Br dropwise within 10 min. at 95-105°, heated 2 hrs., and worked up as usual gave 2.715 g. IV, colorless oil, b<sub>0.04</sub> 110-20°;

free acid, m. 140.5-1.0°. IV (2.197 g.) and 4 cc. Me<sub>2</sub>NPh heated 24 hrs. to 200° in a high vacuum and distilled yielded 1.5 g. 4,2,6-MeO<sub>2</sub>C(CH<sub>2</sub>:CHC<sub>14</sub>H<sub>2</sub>)<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OH, m. 58-9.5° (from C<sub>5</sub>H<sub>12</sub>-C<sub>6</sub>H<sub>6</sub>); Me ether, colorless oil, b<sub>0.01</sub> 105-15°. The corresponding compds., III, b<sub>10</sub> 110-20°, and 4,2,6-Me(CH<sub>2</sub>:CHC<sub>14</sub>H<sub>2</sub>)<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OMe, b<sub>0.05</sub> 70-80°, were prepared similarly.

IT 855945-29-8P, Ammonium, [3-(p-carboxyphenoxy)propyl-1-C<sub>14</sub>]trimethyl-, iodide, Et ester  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 855945-29-8 CAPLUS  
 CN Ammonium, [3-(p-carboxyphenoxy)propyl-1-C<sub>14</sub>]trimethyl-, iodide, Et ester  
 (5CI) (CA INDEX NAME)



● I-

L8 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:46932 CAPLUS

DOCUMENT NUMBER: 45:46932

ORIGINAL REFERENCE NO.: 45:7976h-i,7977a-b

TITLE: Syntheses of basic phenol alkyl ethers. X. Derivatives of isoeugenol, resorcinol, and salicylic acid

AUTHOR(S): Senda, Shigeo

CORPORATE SOURCE: Univ. Kyoto

SOURCE: Yakugaku Zasshi (1950), 70, 561-4

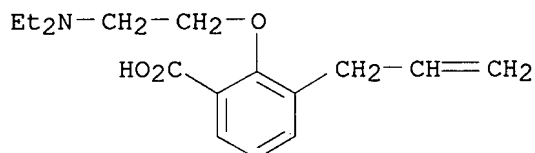
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. preceding abstract The Na salt of isoeugenol and Cl(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub> (I) give 2,4-MeO(MeCH:CH)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub> (II), b<sub>4</sub> 185-7°. Isoeugenol, K<sub>2</sub>CO<sub>3</sub>, and C<sub>3</sub>H<sub>5</sub>Br in Me<sub>2</sub>CO give 2,4-MeO(MeCH:CH)C<sub>6</sub>H<sub>3</sub>OC<sub>3</sub>H<sub>5</sub> (III), b<sub>4</sub> 153°. Heating III at 280-90° in vacuo gives 2,4,6-MeO(MeCH:CH)(C<sub>3</sub>H<sub>5</sub>)C<sub>6</sub>H<sub>2</sub>OH (IV), b<sub>3</sub> 145°. Adding 5.5 g. IV to 0.68 g. Na in 25 ml. MeOH, then 6 g. I, heating at 100° 5 hrs., and distilling gives 1 g. 2,4,6-MeO(MeCH:CH)(C<sub>3</sub>H<sub>5</sub>)C<sub>6</sub>H<sub>2</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub> (V), b<sub>5</sub> 185-8°. Allyl transition by heating 22 g. m-(C<sub>3</sub>H<sub>5</sub>O)<sub>2</sub>C<sub>6</sub>H<sub>4</sub> in vacuo 40 min. at 260-80° gives 9 g. 4,6,1,3-(H<sub>5</sub>C<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>2</sub>(OH)<sub>2</sub> (VI), b<sub>1</sub> 146-7°. Heating 9 g. VI, 2.2 g. Na in 40 ml. MeOH, and 12 g. I on a water bath 7 hrs. and treating as in II gives 5.5 g. 4,6,1,3-(C<sub>3</sub>H<sub>5</sub>)<sub>2</sub>C<sub>6</sub>H<sub>2</sub>(OCH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>)<sub>2</sub> (VII), b<sub>3</sub> 199°. Heating 10 g. 2,3-HO(C<sub>3</sub>H<sub>5</sub>)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Me, 1.2 g. Na in 30 ml. MeOH, and 7 g. I 6 hrs. at 100°, removing the MeOH, acidifying with HCl, taking up with AcOEt, and shaking up with aqueous NaOH gives 6.5 g. 2,6-C<sub>3</sub>H<sub>5</sub>(MeO<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub> (VIII), b<sub>4</sub> 160°; 6-EtO<sub>2</sub>C analog, b<sub>8</sub> 183-5°. Heating 25 g. salicylic acid in 60 ml. acetone with 70 g. K<sub>2</sub>CO<sub>3</sub> and 50 g. C<sub>3</sub>H<sub>5</sub>Br at 100° 8 hrs. and treating as in II gives 3.5 g. 2,6-H<sub>5</sub>C<sub>3</sub>(H<sub>5</sub>C<sub>3</sub>O<sub>2</sub>C)C<sub>6</sub>H<sub>3</sub>O(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub> (IX), b<sub>3</sub> 165°; 2,3-HO(C<sub>3</sub>H<sub>5</sub>)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, b<sub>3</sub> 175°. VIII showed on the uterus of the guinea pig in vivo a contracting action stronger than that of Graviton.

(I. G.) and about the same toxicity on the mouse.  
 IT 860692-96-2, Benzoic acid, 3-allyl-2-(2-diethylaminoethoxy)-  
 (esters)  
 RN 860692-96-2 CAPLUS  
 CN Benzoic acid, 3-allyl-2-(2-diethylaminoethoxy)- (5CI) (CA INDEX NAME)



L8 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1949:36533 CAPLUS

DOCUMENT NUMBER: 43:36533

ORIGINAL REFERENCE NO.: 43:6590d-i, 6591a-g, 6592a-f

TITLE: Synthetic curare compounds. II. Aryl aliphatic derivatives with double quaternary ammonium function

AUTHOR(S): Fusco, Raffaello; Chiavarelli, Stefano; Palazzo, Giuseppe; Bovet, Daniel

SOURCE: Gazzetta Chimica Italiana (1948), 78, 951-64

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 43, 2190d. The purpose was (1) to ascertain the influence on the pharmacodynamic properties of the O bridge which is present in aromatic polyesters and phenolic polyethers and in natural compds. of the tubocurarine group, and (2) to compare the properties of synthetic curare derivs. containing aromatic rings already studied with those of the aliphatic type described by Barlow and Ing (C.A. 42, 6930b), Paton and Zaimis (C.A. 42, 6930d), and Glock, et al. (C.A. 43, 6737b). No previous study has been reported of the pharmacol. properties of aryl aliphatic derivs. with double quaternary ammonium structure. A study of the various methods for preparing p-C6H4(CH2Cl)2 (I) led to the development of the following method as best. PhCH2Cl (1265 g.), 300 g. trioxymethylene, and 1360 g. anhydrous ZnCl2, saturated at 30-40° with HCl, heated at 60° until the exothermic reaction is complete (about 45 min.), then 10 min. at 80°, treated with water, and the C6H6 layer diluted with warm C6H6, washed again with water, distilled to a small volume, and fractionated in vacuo, yields about 400 g. PhCH2Cl; the residue allowed to crystallize ice-cold, and the product (275 g.) washed with petr. ether, and purified by C6H6, EtOH, or ligroin, yields I. I (9 g.) and HNMe2 (approx. 4 mols.) in 100 cc. C6H6 heated in a sealed tube at 60° overnight, taken up in water, NaOH added, and the C6H6 layer dried with NaOH, and distilled in vacuo, yield 7.5 g. (75%) N,N,N',N'-tetramethyl- $\alpha,\alpha'$ -p-xylenediamine, p-C6H4(CH2NMe2)2 (II), b1 102°. I (17.5 g.) and 30 g. HNEt2, refluxed 3 hrs. (until, when diluted with acidified water, the mixture is clear), taken up in water, K2CO3 added, extracted with Et2O, and the extract dried with K2CO3 and distilled in vacuo, yield 17.5 g. (70%) N,N,N',N'-tetraethyl- $\alpha,\alpha'$ -p-xylenediamine (III), b1 110°. Excess MeI added cautiously to II in Me2CO (heat is evolved), and refluxed briefly, yields almost 100% p-xylylenebis-[trimethylammonium iodide] (IV), sinters 286°, m. 298-300° (decomposition). Similarly EtI and II in Me2CO, refluxed 2 hrs., yield almost 100% of p-xylylenebis[ethyldimethylammonium iodide] (V), m. 240-1° (decomposition). MeI and III in Me2CO, refluxed 2 hrs., give, after purification by dilute EtOH, a high yield of p-xylylenebis[diethylmethylammonium iodide] (VI), m. 228-30° (decomposition). It was found impossible to make I react with NEt3; but 8.8 g. I in 70 cc. anhydrous EtOH and 16.7 g.

NaI in 40 cc. anhydrous EtOH, refluxed 30 min., taken up in water, filtered, dried in vacuo, and purified by EtOH, yield 13.5 g. p-C<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>I)<sub>2</sub> (VII), m. 166-9° (cf. Finkelstein, C.A. 4, 2441). VII and 2 mols. NEt<sub>3</sub>, heated in a sealed tube 30 min. at 80°, taken up in EtOH, water added, clarified by animal charcoal, excess NaOH added, and the precipitate purified by EtOH, yield p-xylylenebis[triethylammonium iodide] (VIII), m. 221-2° (decomposition). A very high yield is obtained when it is prepared from III and EtI in Me<sub>2</sub>CO by the foregoing technique. The method of Ruggli, et al. (C.A. 30, 1759.1) for preparing p-C<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>)<sub>2</sub> (IX), b<sub>4</sub> 137-8°, was modified by heating p-C<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>CN)<sub>2</sub>, H, Raney Ni, and alc. NH<sub>3</sub> 15 min. at 90° under 90 atmospheric pressure. IX (2.8 g.) in MeOH, 6 g. KOH in 50 cc. MeOH, and 22 g. MeI, refluxed 1 hr., evaporated, the residue dissolved in hot water, filtered, allowed to stand, and the precipitate washed with MeOH and purified by water, yield 1,4-bis(2-dimethylaminoethyl)benzene-2-MeI (X), m. 314° (decomposition). Similarly 1.6 g. IX and EtI yield 3.1 g. of 1,4-bis(2-diethylaminoethyl)benzene-2EtI (XI), m. 262-3°. IX, KOH, and PrI in PrOH, refluxed 2 hrs., and the product purified by PrOH, yield 1,4-bis(2-dipropylaminoethyl)benzene-2PrI (XII), m. 214-15° (decomposition). 2,4,1,5-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>(CH<sub>2</sub>Cl)<sub>2</sub> (20.5 g.) in 120 cc. MeOH and aqueous NaCN (12.5 g. in 37 cc.), refluxed 30 min., 300 cc. water added, made ice-cold, and the precipitate purified by MeOH and animal charcoal, yield 10 g. of 1,5-dimethyl-2,4-bis(cyanomethyl)benzene (XIII), m. 88-9°. XIII (10 g.) in 150-200 cc. anhydrous EtOH, saturated at 0° with NH<sub>3</sub>, hydrogenated with 1-2 g. Raney Ni at 80-6° and 100 atmospheric pressure (about 1.5 hrs.), and the filtered mixture distilled in vacuo, yields 7 g. of 1,5-dimethyl-2,4-bis(2-aminoethyl)benzene (XIV), b<sub>2</sub> 147°. Following the procedure used in the preparation of XI, 1.9 g. XIV yields 5.5 g. 1,5-dimethyl-2,4-bis(2-diethylaminoethyl)benzene-2EtI (XV), m. 255-6° (decomposition). The following method for preparing 2,4-bis(chloromethyl)anisole (XVI) is an improvement over other published methods. Anisole (100 g.), 142 g. 37% HCHO, and 795 g. concentrated HCl, saturated with HCl (keeping cold by ice-salt), allowed to stand 1 hr. at 10-12°, heated 3 hrs. at 60°, the upper layer poured onto ice, the precipitate dissolved in Et<sub>2</sub>O, washed, dried by CaCl<sub>2</sub>, the Et<sub>2</sub>O distilled, the residue taken up in petr. ether, made ice-cold, and the precipitate purified by petr. ether, yields 104 g. (58%) XVI. XVI (100 g.) and NaCN (calculated weight) in anhydrous MeOH precipitate NaCl; the product, diluted, extracted with a solvent (not specified), and the extracted product fractionated in vacuo, yields in great part a distillate b<sub>2</sub>-3 120-195° and 8.5 g. of impure 2,4-bis(cyanomethyl)anisole (XVII), b<sub>2</sub> approx. 200°. By hydrogenation, 8 g. XVII yields 2,4-bis(2-aminoethyl)anisole (XVIII), b<sub>4</sub> 164°. Ethylation of XVIII is carried out as above, except that the final product is extracted and purified by anhydrous EtOH; the product is 2,4-bis(2-diethylaminoethyl)anisole-2EtI (XIX), m. 236-7° (decomposition). p-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et (8 g.) in alc., NaOEt (from 1.25 g. Na and 30 cc. anhydrous EtOH), and Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl (XX) [from 11 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl.HCl (XXI) by treatment with K<sub>2</sub>CO<sub>3</sub> and extraction with Et<sub>2</sub>O], heated in a sealed tube 24 hrs. at 140°, filtered, evaporated in vacuo, the residue taken up in water, K<sub>2</sub>CO<sub>3</sub> added, extracted with Et<sub>2</sub>O, the extract evaporated, and the residue fractionally distilled in vacuo, give a small yield of Et p-(2-diethylaminoethoxy)-benzoate (XXII), b<sub>2</sub> 168-9°. With EtI, XXII forms the ethiodide, p-IEt<sub>3</sub>NCH<sub>2</sub>CH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et. XXII (6 g.), 5 cc. concentrated HCl, and 40 cc. water, refluxed 8 hrs., concentrated, allowed to stand, and the precipitate purified by aqueous Me<sub>2</sub>CO, yield 5.5 g. p-(2-diethylaminoethoxy)benzoic acid, m. 170-1°. p-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H (3.6 g.)

in a min. of anhydrous EtOH, NaOEt (from 1.25 g. Na and 24 cc. anhydrous EtOH), and XX (from 10 g. XXI), heated in a sealed tube overnight at 130°, filtered, evaporated, the residue taken up in anhydrous Et2O, filtered, evaporated,

and the residue distilled in vacuo, yield XXII. A method different from that of Rohmann and Scheurle (C.A. 30, 4160.7) was used for preparing p-HOC6H4CO2CH2CH2NEt2 (XXIII). HCl gas, passed through 13.8 g. p-HOC6H4CO2H and 11.7 g. Et2NCH2CH2OH (XXIV) at 115-20° for several hrs., taken up in 6 parts by weight of hot EtOH, allowed to cool, and the precipitate purified by EtOH, yields XXIII.HCl (XXV), m. 185-6°. XXV (6 g.) in anhydrous EtOH, EtONa (from 1.25 g. Na and 25 cc. anhydrous EtOH), and

XX

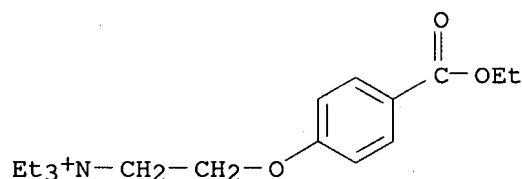
(from 5.5 g. XXI), heated in a sealed tube 48 hrs. at 120°, and the same procedure followed as before, yields 2.6 g. XXII. HCl gas, passed through 7.8 g. XXII and 4 g. XXIV 8 hrs. at 110-20°, taken up in water, K2CO3 added, extracted with Et2O, and the extract dried, evaporated, and distilled in vacuo, yields p-Et2NCH2CH2OC6H4CO2CH2CH2NEt2 (XXVI), b2 190-5°. With excess EtI, and purification of the product by anhydrous EtOH, it yields 2-diethylaminoethyl p-(2-diethylaminoethoxy)benzoate-2EtI, p-IEt3NCH2CH2OC6H4CO2CH2CH2NEt3I (XXVII), m. 175-6° (decomposition). The pharmacol. properties of 10 of the compds. were tested by endovenous injection in rabbits. The following data give the "head-drop" dose (cf. preceding work, loc. cit.) and lethal dose in mg./kg., resp.: IV, 25, 40; V, 15, 15; VI, 8, 15; VIII, 2, 3; X, 20, 25; XI, 3, 4; XII, 10, 12; XV, 2, 3; XIX, 2, 3; XXVII, 4, 15. These results show that, with progressive substitution of Et by Me groups, the curarizing power of any series of compds. decreases, but that neither the position of the chain carrying the ammonium ion nor the number of C atoms which sep. the N from the nucleus has any great influence on the curarizing power. The curarizing power of XXVII is, as expected, of the same magnitude as that of p-C6H4(OCH2CH2NEt3I)2 and p-C6H4(CH2CH2NEt3I)2, which are equally active. Furthermore, this activity is about the same as that of VIII; hence the presence of an oxygenated group has no significant influence on the curarizing power.

IT 857159-93-4P, Ammonium, [2-(p-carboxyphenoxy)ethyl]triethyl-, iodide, Et ester

RL: PREP (Preparation)  
(preparation of)

RN 857159-93-4 CAPLUS

CN Ammonium, [2-(p-carboxyphenoxy)ethyl]triethyl-, iodide, Et ester (5CI)  
(CA INDEX NAME)



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L8 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1949:17410 CAPLUS

DOCUMENT NUMBER: 43:17410

ORIGINAL REFERENCE NO.: 43:3360h-i,3361a-i,3362a-g

TITLE: Biosynthesis of penicillins. V. Substituted

phenylacetic acid derivatives as penicillin precursors

AUTHOR(S): Corse, Joseph W.; Jones, Reuben G.; Soper, Quentin F.; Whitehead, Calvert W.; Behrens, Otto K.

SOURCE: Journal of the American Chemical Society (1948), 70, 2837-43  
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 43, 2274b. A description is given of substituted PhCH<sub>2</sub>CO<sub>2</sub>H derivs. which have been tested as precursor substances in the preparation of new penicillins. p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>Et (I) (36 g.) and 38 g. PhCH<sub>2</sub>Cl in 300 mL. absolute EtOH containing 13.3 g. MeONa, refluxed overnight and the ester refluxed overnight with 70 g. KOH in 400 mL. EtOH and 70 mL. H<sub>2</sub>O, give 15.2 g. (p-benzyloxyphenyl)acetic acid (II), m. 120-1°. I (15.2 g.) in 200 mL. H<sub>2</sub>O and 48.4 mL. 4.135 N NaOH (stirred in an ice bath), treated dropwise with 12 g. ClCO<sub>2</sub>Et, the mixture stirred 2 h., and 32 mL. 4 N HCl added, gives (p-carbomethoxyphenyl)acetic acid, m. 78-9°. II (15.2 g.) in 30 mL. SOCl<sub>2</sub>, the mixture kept overnight, the residue treated with 11.7 g. DL-valine and 16 mL. 12 N NaOH in 200 mL. H<sub>2</sub>O, gives N-(p-benzyloxyphenylacetyl)-DL-valine (III), m. 144-5°, S 1.37 (S is the stimulation; compds. were tested at 0.0008 M concentration; the values represent the ratio units in test container/units in control container). The following analogs of III were prepared (R in RC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHCH(CHMe<sub>2</sub>)CO<sub>2</sub>H) (S is 1 unless otherwise given): o-NO<sub>2</sub> m. 173-5°, m-NO<sub>2</sub> m. 153-8° (S 0.88), p-NO<sub>2</sub> m. 134-5° (S 1.49), o-NH<sub>2</sub> m. 238-41° (S 1.37), p-NH<sub>2</sub> m. 220-7° (prepared by catalytic reduction of the NO<sub>2</sub> derivs.), o-Cl m. 122-4°, p-Cl m. 144-5° (S 1.33), p-CN m. 138-40° (S 1.24), p-I m. 148-50°, p-iso-Pr m. 114-15°, p-MeO m. 129° (S 1.52), 2,4,6-tri-Me m. 130-2° N-(p-nitrophenylacetyl)isoleucine m. 113-15°. The following esters were prepared by treating the substituted PhMe with Br and the resulting PhCH<sub>2</sub>Br with KCN, hydrolyzing the nitrile with aqueous alc. H<sub>2</sub>SO<sub>4</sub>, and esterifying with MeOH-H<sub>2</sub>SO<sub>4</sub>: Me (3,4-dibromophenyl)acetate m. 44-5° 3,4,5-tri-Br analog m. 78-9° 4-bromo-3-chloro analog m. 42-3°. Et (o-fluorophenyl)acetate, b<sub>24</sub> 135-6°, 52%; m-isomer, b<sub>28</sub> 126-9°, 22%; p-isomer, b<sub>31</sub> 128-30°, n<sub>25D</sub> 1.4776, 48%. Et (4-amino-3-nitrophenyl)acetate, bright yellow, m. 80-1° (68% on saturating the acid in EtOH with HCl and standing overnight). 3,4-MeO(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>Cl through the nitrile yields (4-methoxy-3-nitrophenyl)acetic acid, m. 122-5°. MeSPh (24.8 g.), 150 mL. CS<sub>2</sub>, and 24 g. AcCl at 0°, treated with 30 g. AlCl<sub>3</sub> (in portions) and the mixture stirred 4 h., give p-methylmercaptoacetophenone (III), m. 72-5° 49.8 g. III, 9.6 g. S, and 27 mL. morpholine, refluxed overnight, treated with 400 mL. concentrated HCl and 300 mL. H<sub>2</sub>O, and again refluxed overnight, give 25 g. (p-methylmercaptophenyl)acetic acid, m. 92-4° Me ester b<sub>3</sub> 179-81°. m-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>CN (51.5 g.) in 50 mL. ether, added (1 h.) to MeMgI (60 g. MeI) and, after 3 h., poured into 500 g. ice and 100 mL. concentrated HCl, gives 50% m-(trifluoromethyl)acetophenone (IV), b. 198-200°. m-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>COC<sub>2</sub>H<sub>5</sub> (b<sub>750</sub> 184-6°, 95.5% yield) (93.5 g.) in 100 mL. ether, added dropwise to CdMe<sub>2</sub> (25 mg. Mg, 100 g. MeBr, and 110 g. CdCl<sub>2</sub>) in 700 mL. ether, gives 91% IV. IV (10 g.), 2 g. S, and 5.3 g. morpholine, heated 16 h. at 135°, treated with 30 mL. AcOH and 50 mL. concentrated HCl, and refluxed 7 h., give 89% [m-(trifluoromethyl)phenyl]acetic acid, m. 72-3°. p-PhOC<sub>6</sub>H<sub>4</sub>Ac (60 g.), 13 g. S, and 10 mL. morpholine, refluxed overnight, the crude product hydrolyzed (2 days) by refluxing with 75 g. KOH in 75 mL. H<sub>2</sub>O and 600 mL. EtOH, and the acid esterified with EtOH and H<sub>2</sub>SO<sub>4</sub>, give 25 g. Et (p-phenoxyphenyl)acetate, b<sub>0.2</sub> 173-4°. p-MeOC<sub>6</sub>H<sub>4</sub>CONHC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H (m. 211-12°) and excess CH<sub>2</sub>N<sub>2</sub> in MeOH-ether give a quant. yield of the Me ester, m. 162°.

Ph<sub>2</sub>S and AcCl give p-phenylmercaptoacetophenone, b<sub>1</sub> 180°, which, by the Willgerodt method and esterification, yields Et (p-phenylmercaptophenyl)acetate, b<sub>0.65</sub> 163°. I (36 g.) in 300 mL. absolute EtOH containing 11 g. MeONa, refluxed overnight with 30 g. Et<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>Cl, gives 24 g. Et [p-(3-diethylaminopropoxy)phenyl]acetate, b<sub>0.3</sub> 145-7° (HCl salt, m. 121°).

p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHCH<sub>2</sub>CH<sub>2</sub>OH (V) (49 g.) in 165 mL. 10% NaOH, treated with PhN<sub>2</sub>Cl (23 g. PhNH<sub>2</sub>) at 0°, gives 56.5 g. N-2-hydroxyethyl-α-(4-hydroxy-3-phenylazophenyl)acetamide, m. 180-1.5°. V (49 g.) and 79.7 g. Hg(OAc)<sub>2</sub> in 800 mL. 50% EtOH and 40 mL. AcOH, allowed to stand 12 days at room temperature and the solid product heated with 750 mL. 50% EtOH containing 5% AcOH, gives 51.4 g. N-2-hydroxyethyl-α-[3,5-bis-(acetylmercuri)-4-hydroxyphenyl]acetamide, partially m. at 240° (rapid heating). p-tert-BuC<sub>6</sub>H<sub>4</sub>Ac (87 g.) through the acid (Willgerodt method), yields 19.4 g. Et (p-tert-butylphenyl)acetate, b<sub>0.47</sub> 95°.

p-tert-AmC<sub>6</sub>H<sub>4</sub>Ac (68.5 g.) yields 15 g. Et (p-tert-amylphenyl)acetate, b<sub>2</sub> 124°. Reaction of I (90 g.) and 70 g. CH<sub>2</sub>:CHCH<sub>2</sub>Br, followed by esterification, gives 18.4 g. Et (p-allyloxyphenyl)acetate (VI), b<sub>0.5</sub> 126-7° oxidation of 44 g. VI in 100 mL. 70% Me<sub>2</sub>CO with 22 g. KMnO<sub>4</sub> in 300 mL. 70% Me<sub>2</sub>CO (with addition of 8 g. AcOH to the mixture) yields 24.8 g. Et [p-(2,3-dihydroxypropoxy)phenyl]acetate, b<sub>0.2</sub> 200°.

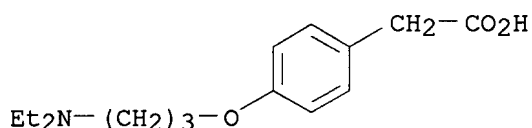
N-2-Hydroxyethyl amides, RC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHCH<sub>2</sub>CH<sub>2</sub>OH, were prepared by heating the above and other esters with excess H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH overnight on the steam bath or several hrs. at 110-20° (R given; S is 1 unless otherwise given): p-acetamido m. 145-6°, p-allyloxy m. 84-5° (S 1.23), 4-amino-3-nitro m. 132°, p-NH<sub>2</sub> m. 103-4° (S 1.14), p-tert-Am oil, p-anisoylamino m. 210-11°, 4-bromo-3-chloro m. 104-6° (S 1.71), o-Br m. 106-7°, m-Br m. 129-30° (S 2.21), p-Br m. 108-9° (S 2.90), p-tert-Bu, oil, o-Cl m. 99-100°, m-Cl m. 114-17° (S 1.84), p-Cl m. 90-1° (S 1.97), 3,5-bis(acetylmercuri)-4-hydroxy, 3,5-dibromo-4-hydroxy m. 200-2°, 3,4-di-Br m. 125-7°, 2,4-di-Cl m. 118-19°, 3,4-di-Cl m. 113-14° (S 2.10), p-(3-diethylaminopropoxy) oil, p-(2,3-dihydroxypropoxy) oil (S 1.20), 3,5-diiodo-4-hydroxy m. 179-80°, 2,3-di-MeO m. 93°, 3,4-di-MeO m. 96-8°, 3,4-di-Me m. 99-100° (S 1.27), p-EtO m. 90-1° (S 1.26), o-F m. 103-5° (S 1.23), m-F m. 75-7° (S 1.93), p-F m. 75° (S 1.54), o-HO oil (S 1.24), m-HO m. 92-3° (S 1.13), p-HO m. 110-12°, p-(2-hydroxyethylcarbonyl) m. 157-8°, 4-hydroxy-3-phenylazo m. 180-1.5°, m-I m. 127-9° (S 1.75), p-I m. 112-13° (S 1.83), 5-isopropyl-2-Me oil, p-iso-Pr oil (S 1.33), o-MeO oil, m-MeO m. 59°, p-MeO m. 86-8° (S 1.22), 3,4-methylenedioxy m. 99-100°, p-methylmercapto m. 115-17° (S 1.49), 4-methoxy-3-nitro m. 69°, o-Me m. 63-4° (S 1.36), m-Me oil (S 1.39), p-Me m. 76-8° (S 1.69), p-NO<sub>2</sub> m. 140-2°, p-PhO m. 95° (S 1.64), p-phenylmercapto m. 89-90°, p-Ph m. 172-5° (S 0.87), 3,4,5-tri-Br m. 212-13° (S 0.33), m-F<sub>3</sub>C oil (S 1.28), 2,4,6-tri-Me m. 144-5°. N-Allyl-α-(p-hydroxyphenyl)acetamide m. 84-6°. N-(2-Aminoethyl)-α-(p-methoxyphenyl)acetamide-HCl m. 135-8° (S 1.34). PhCH<sub>2</sub>CS<sub>2</sub>Me (18.2 g.) in 15 g. MePrNH on heating to boiling gives 86% N-methyl-N-propyl-α-phenylthioacetamide, b<sub>1.5</sub> 155-8°, n<sub>24.5D</sub> 1.5876. The following phenylthioacetyl derivs. were prepared by exactly neutralizing the amino acid with 4 N NaOH, diluting with an equal volume of EtOH, adding 10% molar excess PhCH<sub>2</sub>CS<sub>2</sub>Me, and shaking for a few min. to several hrs.: D-penicillamine m. 132-3°, 55%; L-isomer m. 133-4°, 61%; β,β-diethoxyalanine, with 0.5 mol. H<sub>2</sub>O, m. 67.5-8°, 84%; DL-valine m. 102-3°, 95%; DL-isoleucine m. 95-6°, 75%. Details are given of the formation of p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHCH<sub>2</sub>CH<sub>2</sub>OH. From the results of the S data it is difficult to draw any generalizations. Both the kind and position of the

substituents had a marked influence upon the ability of the compound to act as a penicillin precursor. That the nature of the PhCH<sub>2</sub>CO<sub>2</sub>H derivative had a profound influence upon its utilization by the mold was illustrated in several cases.

IT 861065-20-5P, Acetic acid, [p-(3-diethylaminopropoxy)phenyl]-, hydrochloride  
RL: PREP (Preparation)

(preparation of)  
RN 861065-20-5 CAPLUS

CN Acetic acid, [p-(3-diethylaminopropoxy)phenyl]-, hydrochloride (5CI) (CA INDEX NAME)



● HCl

L8 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1947:814 CAPLUS

DOCUMENT NUMBER: 41:814

ORIGINAL REFERENCE NO.: 41:155c-i,156a-i,157a-g

TITLE: Amino alcohol esters of hydroxybenzoic acids

INVENTOR(S): Christiansen, Walter G.; Harris, Sidney E.

PATENT ASSIGNEE(S): E. R. Squibb & Sons

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2404691		19460723	US	<--

GI For diagram(s), see printed CA Issue.

AB Amino alc. esters of hydroxybenzoic acids, effective for inducing local anesthesia and having the general formula in which R is a bivalent aliphatic, cycloaliph., or aromatic radical providing a continuous C bridge, R' and R'' represent alkyl, aralkyl, hydroxyalkyl, or hydroxyaralkyl, or jointly represent an alkylene group, R''' represents an aliphatic, aromatic, or araliph. radical, R'''' represents H, alkyl, or an alkoxy radical, and Y is H or alkyl, are prepared by treating an aracyl halide with an amino alc. p-EtOC<sub>6</sub>H<sub>4</sub>COCl (10 g.) in 50 cc. dry benzene is treated with 6.8 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH. A precipitate forms, and the reaction is completed by heating on the H<sub>2</sub>O bath. The solution is cooled, the precipitate is filtered and treated with a slight excess of 2 N KOH, and the ester is extracted with Et<sub>2</sub>O and dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>. The Et<sub>2</sub>O solution is treated with dry HCl, and the precipitate is filtered and washed with dry Et<sub>2</sub>O to yield 2-diethylaminoethyl p-ethoxybenzoate-HCl, m. 172.5-3.5°. p-EtOC<sub>6</sub>H<sub>4</sub>COCl (4.1 g.) in 15 cc. dry benzene is refluxed 30 min. with 3.5 g. AmNEtCH<sub>2</sub>CH<sub>2</sub>OH in 10 cc. dry benzene. The benzene is distilled in vacuo and the residue is dissolved in EtOH, decolorized with C, repptd. with dry Et<sub>2</sub>O, and recrystd. from Me<sub>2</sub>CO-petr. ether to give 2-(ethylamylamino)ethyl p-ethoxybenzoate-HCl, m.

108-10°. By processes essentially similar to the above described ones were prepared 2-dibutylaminoethyl p-ethoxybenzoate-HCl, m. 144.5-5.5°; 3-dibutylaminopropyl p-ethoxybenzoate-HCl, m. 85.6-6.6°; 2-diethylaminoethyl p-butoxybenzoate-HCl, m. 146°; 2-diethylaminoethyl 2-ethoxy-3-methylbenzoate-HCl, m. 97-7.5°; 2-diethylaminoethyl p-butoxybenzoate-HCl, m. 132-3°; 2-diethylaminoethyl o-ethoxybenzoate-HCl, m. 139-9.5°; 2-diethylaminoethyl p-(2-diethylaminoethoxy)benzoate-HCl, hygroscopic crystals, m. 143°; 2-diethylaminoethyl 2-methyl-4-ethoxybenzoate-HCl, m. 101-3°; 2-diethylamino-Et 3-methyl-4-ethoxybenzoate-HCl, m. 142.5-5°; 2-diethylaminoethyl p-(2-bromallyloxy)benzoate-HCl, m. 81.5-3.5°; and 2-diethylaminoethyl 3-methoxy-4-ethoxybenzoate-HCl, m. 171.5-2.5°. A mixture of 5.5 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OH, 9.3 g. p-EtOC<sub>6</sub>H<sub>4</sub>COCl and 25 cc. 10% NaOH solution is vigorously stirred 0.5 h., cooled, and extracted with benzene. The benzene solution is washed with dilute NaOH and H<sub>2</sub>O, and distilled. The residual oil is dissolved in absolute alc. HCl and diluted with Et<sub>2</sub>O. The precipitate

is filtered and recrystd. from EtOH-Et<sub>2</sub>O to give 3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 148.5-9.5°. 2-Diethylaminocyclohexanol (6.8 g.) in 75 cc. dry benzene is treated with 10 g. finely powdered anhydrous K<sub>2</sub>CO<sub>3</sub> and then with 7.3 g. p-EtOC<sub>6</sub>H<sub>4</sub>COCl. The mixture is refluxed several hrs. and treated with 100 cc. H<sub>2</sub>O and 100 cc. benzene. The benzene layer is removed and purified and treated as in the above preparation to yield 2-diethylaminocyclohexyl p-ethoxybenzoate-HCl, m. 184-5°. In substantially the same manner were prepared 2-hydroxy-3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 120-6°; and (N-phenacyl-N-ethylamino)ethyl p-ethoxybenzoate-HCl, white crystals. (HOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NEt (6.7 g.) in 100 cc. dry benzene is treated with 14 g. anhydrous K<sub>2</sub>CO<sub>3</sub> and then with 9.2 g. p-EtOC<sub>6</sub>H<sub>4</sub>COCl, and the mixture is refluxed with stirring for 2 h. The mixture is filtered, the benzene evaporated, and the residue distilled in vacuo to yield

2-[ethyl(2-hydroxyethyl)amino]ethyl p-ethoxybenzoate, thick, colorless oil, b<sub>8</sub> 218-25°; HCl salt, hygroscopic crystals. In similar manner were prepared 2-diethylaminoisohexyl p-ethoxybenzoate, b<sub>2.5</sub> 175-85°, b<sub>5</sub> 193-5°; 3-diethylamino-2-hydroxypropyl p-butoxybenzoate-HCl, mixture of 2 isomers, m. 79-96°; 2-[ethyl(2-hydroxyethyl)amino]ethyl p-butoxybenzoate, b<sub>3</sub> 216-20°; HCl salt, hygroscopic. A mixture of 1.5 g. Me<sub>2</sub>NCH<sub>2</sub>CEt(OH)CH<sub>2</sub>NMe<sub>2</sub> in 5 cc. CHCl<sub>3</sub> and 1.6 g. p-EtOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H in 5 cc. CHCl<sub>3</sub> is heated 5 min. on the steam bath. Dry Et<sub>2</sub>O is added, and the precipitate is filtered, washed, and dried to give 1,1-bis(dimethylaminomethyl) Pr p-ethoxybenzoate-HCl, white crystalline powder, m. 121-1.5°. In like manner was prepared 1,1-bis(dimethylaminomethyl)propyl p-butoxybenzoate-HCl, m. 111°. m-EtOC<sub>6</sub>H<sub>4</sub>COCl (11.5 g.) in 50 cc. dry benzene is mixed with 14.5 Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH in 50 cc. dry benzene, and the mixture heated on the steam bath 1 h. The precipitate is filtered, and the benzene filtrate is distilled. The residue is distilled in vacuo to give 2-diethylaminoethyl m-ethoxybenzoate, b<sub>2</sub> 163-75°. This was dissolved in alc. HCl, and reprecipitated with Et<sub>2</sub>O to yield the HCl salt, m. 125-5.5°. Similarly were prepared 2-diethylaminoethyl p-(2-ethoxyethoxy)benzoate-HCl, m. 102-3.5°; 2-diethylaminoethyl p-propoxybenzoate, b<sub>4</sub> 160-5° (HCl salt, m. 135-6°); 2-diethylaminoethyl p-isopropoxybenzoate-HCl, m. 125.5°; and 2-diethylaminoethyl p-allyloxybenzoate, b<sub>4</sub> 165-75° (HCl salt, m. 130°). A mixture of 2.5 g. p-EtOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH:CHBr, 5.5 g. Et<sub>2</sub>NH, and 15 cc. benzene is heated in a sealed tube at 125-35° for 8 h. After cooling, the mixture is treated with H<sub>2</sub>O and extracted with Et<sub>2</sub>O. The Et<sub>2</sub>O extract is washed with H<sub>2</sub>O, dried, and distilled on the steam bath, finally under reduced pressure. The residue is dissolved in alc. HCl and precipitated with Et<sub>2</sub>O. Washing with dry Et<sub>2</sub>O of the oily precipitate yields 4-diethylamino-4-butenyl p-ethoxybenzoate-HCl, yellowish white crystals, m. 146-7°. Heating Et<sub>2</sub>NCH<sub>2</sub>CMe<sub>2</sub>CH<sub>2</sub>OH

with p-EtOC<sub>6</sub>H<sub>4</sub>COCl in dry Me<sub>2</sub>CO yields 2,2-dimethyl-3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 122-4°. 3,4-Me (BuO)C<sub>6</sub>H<sub>3</sub>COCl (1.05 g.) and 1.25 g. (Me<sub>2</sub>NCH<sub>2</sub>)<sub>2</sub>C(OH)CH<sub>2</sub>CH<sub>2</sub>Ph in 10 cc. CHCl<sub>3</sub> are refluxed for a few min., treated with dry Et<sub>2</sub>O to incipient precipitation, and allowed to stand.

The

crystalline precipitate which seps. after some time is filtered and washed with dry

Et<sub>2</sub>O to give 1,1-bis(dimethylaminomethyl)-3-phenylpropyl 3-methyl-4-butoxybenzoate-HCl, m. 161-2°. Similarly were prepared 2,2'-bis(dimethylamino)isopropyl p-propoxybenzoate mono- and di-HCl salts, m. 208°; 3-dimethylaminopropyl 3-methyl-4-butoxybenzoate-HCl, white crystalline powder, m. 125.5-6.5°; 3-dimethylaminopropyl p-(2-phenylethoxy)benzoate-HCl, m. 156.5-7-5°; and 1-methyl-1-(dimethylaminomethyl)amyl 3-methyl-4-butoxybenzoate-HCl, m. 126-31°. p-EtOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NEtCH<sub>2</sub>COPh (0.9 g.) in 60 cc. EtOH containing 0.3 g. PtO is shaken 8 h. under a pressure of 35 lb. H, filtered, and the filtrate is concentrated to a small volume and diluted with Et<sub>2</sub>O. The crystalline precipitate is filtered, washed with Et<sub>2</sub>O, and dried in vacuo over

CaCl<sub>2</sub>

to give 2-[ethyl(2-phenyl-2-hydroxyethyl)amino]ethyl p-ethoxybenzoate-HCl. 2-Diethylaminoethyl p-(p-aminobenzyloxy)benzoate-HCl, m. 185-7°, is prepared in the same manner, p-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub> (0.4 g.) in 50 cc. dry Me<sub>2</sub>CO containing 15 g. anhydrous K<sub>2</sub>CO<sub>3</sub> is treated with 5.5 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>Br, and the mixture is refluxed 12 h. The mixture is filtered, and the Me<sub>2</sub>CO distilled from the filtrate. The residue is treated with alc. HCl and diluted with Me<sub>2</sub>CO and Et<sub>2</sub>O. The

precipitate

is recrystd. from Me<sub>2</sub>CO-Et<sub>2</sub>O to give 2-diethylaminoethyl p-(p-nitrobenzyloxy)benzoate-HCl, m. 145-6°. In addition, 21 other similar compds. are cited, but no phys. properties are recorded. The preps. of many intermediates used in preparing the above compds. are described. A solution of 3.5 g. Na in 100 cc. absolute EtOH is treated first with 25 g. 2,3-HO(MeO)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>Et and then with 20 g. EtBr, and the solution is boiled until neutral to moist litmus. The mixture is filtered, and the EtOH is removed from the filtrate. The residue is fractionated to yield Et 2-ethoxy-3-methylbenzoate, b<sub>6</sub> 116-18°, which upon hydrolysis with alc. NaOH yielded 2-ethoxy-3-methylbenzoic acid, oily precipitate, which was extracted with ether. The ether was removed and the residue treated with SOCl<sub>2</sub> to give 2-ethoxy-3-methylbenzoyl chloride, b<sub>2.5</sub> 102-5°. p-(2-Phenylethoxy)benzoic acid, white powder, m. 163-4° (chloride, b<sub>5</sub> 215-30°), and 3-methyl-4-(2-phenylethoxy)benzoic acid, m. 150-2° (chloride, b<sub>1</sub> 210-15°), were prepared in essentially the same manner. p-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me (13 g.) in 35 cc. Me<sub>2</sub>CO is treated with 15 g. anhydrous K<sub>2</sub>CO<sub>3</sub>, the mixture is refluxed and stirred, treated with 13 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl, heated, stirred 15 h., filtered, and the filtrate concentrated by distillation. The residue is treated with excess NaOH

and

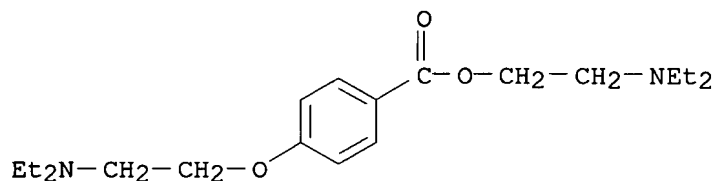
boiled until saponification is complete. The solution is extracted with Et<sub>2</sub>O, and the

aqueous solution is evaporated to dryness in vacuo. The residue is extracted with absolute

EtOH, the extract filtered, the filtrate evaporated to dryness, and the residue recrystd. from MeOHEt<sub>2</sub>O to give p-(2-diethylaminoethoxy)benzoic acid-HCl, white needles, m. 160-1°. Treatment with PCl<sub>5</sub> yields p-(2-diethylaminoethoxy)benzoyl chloride-HCl, m. 143°. In similar manner were prepared 2-methyl-4-ethoxybenzoyl chloride, colorless liquid, b<sub>3</sub> 138-40°; 3-methyl-4-ethoxybenzoyl chloride, colorless liquid, b<sub>6</sub> 147-52°; p-(2-ethoxyethoxy)benzoic acid, m. 131-2° (chloride, b<sub>5</sub> 150-60°); p-(2-bromoallyloxy)benzoic acid, m. 200° (decomposition) (chloride, b<sub>5</sub> 160-70°); 3-methoxy-4-ethoxybenzoyl chloride, b<sub>5</sub> 147-50°, m. 72°, and 3-methyl-4-butoxybenzoic acid, white plates from 60% EtOH, m.

144-6° (chloride, b1.5 144-54°). A mixture of 5.5 g. dry p-EtOC6H4CO2Na, 8 g. BrCH:CHCHBrMe, and 10 g. dry xylene is heated in a sealed tube at 165-70° for 6 h. The contents of the tube are extracted with dilute EtOH and Et2O. The Et2O is washed with H2O, dried over Na2SO4, and distilled. The oily residue is fractionated in a high vacuum to yield 3-bromo-1-butenyl p-ethoxybenzoate, b3 165-75°. A mixture of 9.95 g. PhCOCH2Cl, 4.4 g. EtNHCH2CH2OH, and 100 cc. benzene is refluxed 3 h. On adding 10 g. K2CO3, a vigorous evolution of CO2 ensues. The suspension is further refluxed 4 h. and filtered. The filtrate is treated with HCl in Et2O. The reddish brown semisolid which seps. is filtered, washed with Et2O, and dried in a vacuum over CaCl2 to yield the very hygroscopic N-phenacyl-N-ethyl-2-aminoethanol-HCl, which is treated with p-EtOC6H4COCl in benzene in the presence of K2CO3 in the regular manner to give N-phenacyl-N-ethyl-2-aminoethyl p-ethoxybenzoate-HCl, white crystals.

IT 855470-53-0P, Benzoic acid, p-(2-diethylaminoethoxy)-, 2-diethylaminoethyl ester, hydrochloride  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 855470-53-0 CAPLUS  
 CN Benzoic acid, p-(2-diethylaminoethoxy)-, 2-diethylaminoethyl ester, -HCl (4CI) (CA INDEX NAME)

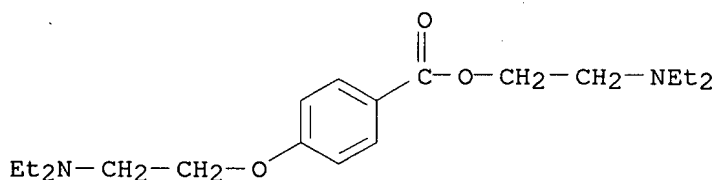


● HCl

L8 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1938:59916 CAPLUS  
 DOCUMENT NUMBER: 32:59916  
 ORIGINAL REFERENCE NO.: 32:8391e-h  
 TITLE: The relation between chemical constitution and local-anesthetic activity. II. Some alkoxybenzoates of di-alkylamino alcohols  
 AUTHOR(S): Lott, W. A.; Harris, S. E.; Christiansen, W. G.  
 SOURCE: Journal of the American Pharmaceutical Association (1912-1977) (1938), 27, 661-5  
 CODEN: JPAA3; ISSN: 0003-0465  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The HCl salts of the diethylaminoethyl esters of the following alkoxybenzoic acids were prepared: p-methoxy, m. 142°; p-ethoxy, m. 177.3°; p-propoxy, m. 137.6-8.1°; p-isopropoxy, m. 125.5°; p-butoxy, m. 146.5-7.5°; p-allyloxy, m. 130°; p-β-phenylethoxy, m. 91-2°; p-β-ethoxyethoxy, m. 102-3.5°; p-β-bromoallyloxy, m. 81.5-3.5°; p-β-diethylaminoethoxy, hygroscopic; o-ethoxy, m. 139-9.5°; m-ethoxy, m. 125-5.5°. The p-ethoxybenzoic ester HCl salts of the following alkylamino alcs. were prepared: ethylamylaminoethyl, m. 108-10°; β-dibutylaminoethyl, m. 144.5-5.5°; γ-dibutylaminopropyl, m. 85.5-6.5°; β,β-dimethyl-γ-diethylaminopropyl, m. 121-1.5°; γ-

diethylaminopropyl, m. 149.9-50.4°; β-diethylamino-δ-methylamyl, oil; α,α-bis(dimethylaminomethyl)propyl, m. 121-1.5°; α-methyl-α-diethylaminomethylpropyl, m. 122-4°; β-diethylaminoethoxyethyl, m. 112-15°; 2-diethylaminocyclohexyl, m. 184-5°; 1-diethylamino-2,3-propanediol, m. p. indefinite; N-ethyldiethanolamine, oil. The p-butoxybenzoic ester HCl salts of the following alkylamino alcs. were prepared; N-ethyldiethanolamine, m. 79.6°; 1-diethylamino-2,3-propanediol, m. p. indefinite; β-dimethylaminoethyl, m. 132-3°. These compds. all proved to be local anesthetics in preliminary pharmacol. tests, details of which will be published shortly.

IT 855470-53-0P, Benzoic acid, p-(2-diethylaminoethoxy)-, 2-diethylaminoethyl ester, -HCl  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 855470-53-0 CAPLUS  
 CN Benzoic acid, p-(2-diethylaminoethoxy)-, 2-diethylaminoethyl ester, -HCl  
 (4CI) (CA INDEX NAME)



● HCl

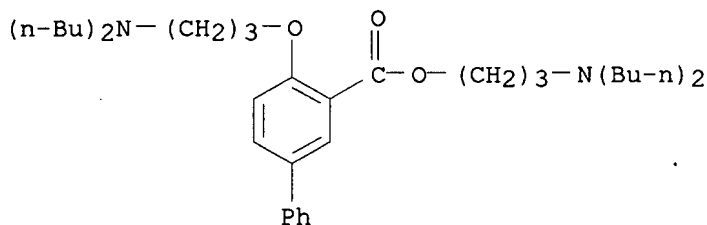
L8 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1934:60903 CAPLUS  
 DOCUMENT NUMBER: 28:60903  
 ORIGINAL REFERENCE NO.: 28:7429h-i,7430a-b  
 TITLE: Dialkylaminoalkyl esters of hydroxy-3-carboxybiphenyls  
 INVENTOR(S): Christiansen, Walter G.; Harvey, Adelbert W.  
 PATENT ASSIGNEE(S): E. R. Squibb & Sons  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 1976922	----	19341016	US	----

AB Compds. (suitable for use as local anesthetics in solution buffered with a phosphate) such as the dialkylaminoalkyl esters of 3 - carboxy - 4 - hydroxybiphenyl and 3 - carboxy - 2-hydroxybiphenyl and salts thereof, particularly 3-β-diethylaminocarbethoxy-4-hydroxybiphenyl and its salts are prepared by converting the hydroxy-3-carboxybiphenyl to a salt, forming a halide ester, preferably a bromoalkyl ester from the salt and then forming the dialkylaminoalkyl ester from this. Purification of the 3-β-diethylaminocarbethoxy-4-hydroxybiphenyl hydrochloride may be accomplished by crystallization from absolute EtOH. The product, in the form of the hydrochloride, is a white crystalline substance soluble in water, m. 167-168.5°. The free ester is an almost colorless oil. Starting with 3-carboxy-2-hydroxybiphenyl and employing similar reactions,

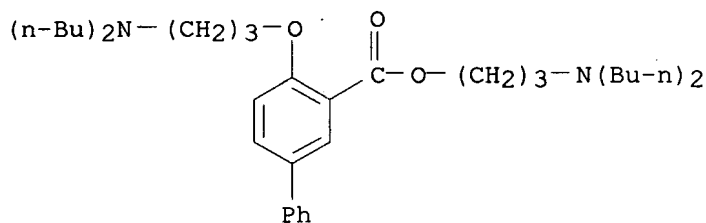
corresponding alkyl derivs. may be formed in which the hydroxy group is in the 2- instead of the 4-position.

IT 873986-35-7, Benzoic acid, 2-( $\gamma$ -dibutylaminopropoxy)-5-phenyl-,  $\gamma$ -dibutylaminopropyl ester  
(and salts)  
RN 873986-35-7 CAPLUS  
CN Benzoic acid, 2-( $\gamma$ -dibutylaminopropoxy)-5-phenyl-,  
 $\gamma$ -dibutylaminopropyl ester (3CI) (CA INDEX NAME)



L8 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1934:60902 CAPLUS  
DOCUMENT NUMBER: 28:60902  
ORIGINAL REFERENCE NO.: 28:7429g-h  
TITLE: Dialkylaminoalkyl esters of dialkylaminoalkoxy-3-carboxybiphenyl  
INVENTOR(S): Christiansen, Walter G.; Braker, William  
PATENT ASSIGNEE(S): E. R. Squibb & Sons  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	US 1976921		19341016	US	<--
AB	Compds. (suitable for use in the preparation of local anesthetics) such as 3- $\beta$ -diethylaminocarbethoxy-4- $\beta$ -diethylaminoethoxybiphenyl and 3- $\gamma$ -dibutylaminocarbopropoxy - 4 - $\gamma$ - dibutylaminopropoxybiphenyl are prepared from a hydroxy-3-carboxybiphenyl by forming its di-Na derivative and then replacing the Na atoms by dialkylaminoalkyl radicals (various details for preparing these compds. and their hydrochlorides and borates being given).				
IT	873986-35-7, Benzoic acid, 2-( $\gamma$ -dibutylaminopropoxy)-5-phenyl-, $\gamma$ -dibutylaminopropyl ester (and salts)				
RN	873986-35-7 CAPLUS				
CN	Benzoic acid, 2-( $\gamma$ -dibutylaminopropoxy)-5-phenyl-, $\gamma$ -dibutylaminopropyl ester (3CI) (CA INDEX NAME)				



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L8 28 S L7 AND PHENYL?

=> s l7 and not l8

MISSING TERM 'AND NOT'

The search profile that was entered contains a logical operator followed immediately by another operator.

=> s l7 not l8

L9 53 L7 NOT L8

=> d 1-53 ibib abs hitstr

L9 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:633275 CAPLUS  
DOCUMENT NUMBER: 139:169333  
TITLE: Novel anticholesterol compositions and method for using same  
INVENTOR(S): Dudley, Robert; Liao, Shutsung; Song, Ching  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 13 pp., Cont.-in-part of U.S. Ser. No. 137,695.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 9  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003153541	A1	20030814	US 2002-174934	20020619
WO 9922728	A1	19990514	WO 1998-US23041	19981030 <--
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CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6576660	B1	20030610	US 2000-530443	20000428
US 6645955	B1	20031111	US 2000-560236	20000428
ZA 2001009793	A	20030228	ZA 2001-9793	20011128
CA 2438221	A1	20020815	CA 2002-2438221	20020207
AU 2002238093	A1	20020819	AU 2002-238093	20020207
EP 1385868	A2	20040204	EP 2002-704407	20020207
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JP 2005508281	T	20050331	JP 2002-562310	20020207
US 2002107233	A1	20020808	US 2002-72128	20020208
US 2002193357	A1	20021219	US 2002-137695	20020502
US 7012069	B2	20060314		
CA 2489702	A1	20031231	CA 2003-2489702	20030619
WO 2004001002	A2	20031231	WO 2003-US19515	20030619
WO 2004001002	A3	20040506		
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AU 2003245605	A1	20040106	AU 2003-245605	20030619
EP 1534298	A2	20050601	EP 2003-739234	20030619
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JP 2005533810	T	20051110	JP 2004-516031	20030619

PRIORITY APPLN. INFO.:

	US 1997-63770P	P	19971031
	WO 1998-US23041	W	19981030
	US 1999-131728P	P	19990430
	US 2000-530443	A2	20000428
	US 2000-560236	A2	20000428
	US 2001-267493P	P	20010208
	US 2001-288643P	P	20010503
	US 2001-348020P	P	20011108
	US 2002-72128	A2	20020208
	US 2002-137695	A2	20020502
	US 2000-191864P	P	20000324
	WO 2002-US3826	W	20020207
	US 2002-174934	A	20020619
	WO 2003-US19515	W	20030619

OTHER SOURCE(S): MARPAT 139:169333

AB Disclosed are compns., methods, combinations, and kits for treating a disorder related to elevated serum cholesterol concentration, for example, atherosclerosis, elevated LDL plasma levels, low HDL plasma levels, hypertriglyceridemia, hyperlipidemia, hypertension, hypercholesterolemia, cholesterol gallstones, lipid storage diseases, obesity, and diabetes. The compns., methods, combinations, and kits of the present invention are pharmaceutical compns. comprising at least two of an LXR receptor modulator, a therapeutically effective amount of a catechin, and/or a therapeutically effective amount of a lipid regulating agent, such as a HMG-CoA reductase inhibitor, a fibric acid derivative, niacin, a bile-acid sequestrant, an absorption inhibitor, probucol, raloxifene and its derivs., an azetidinone compound, and an unsatd. omega-3 fatty acid.

IT 405911-09-3, GW3965

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(anticholesterol compns. containing LXR modulators and lipid regulating agents)

RN 405911-09-3 CAPLUS

CN Benzeneacetic acid, 3-[3-[[[2-chloro-3-(trifluoromethyl)phenyl]methyl](2,2-diphenylethyl)amino]propoxy]- (CA INDEX NAME)

